LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM043403.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.387	30	34	46	rVB	147392	205134	0.18%	0.042%
2	3.669	79	82	95	rBV	165856	275115	0.25%	0.056%
3	3.811	102	106	125	rBV	1504124	2301052	2.05%	0.471%
4	4.034	136	144	150	rBV	172085	287369	0.26%	0.059%
5	5.299	349	359	375	rBV3	50232944	112123320	100.00%	22.947%
6	7.151	667	674	686	rVB	2398318	3883626	3.46%	0.795%
7	7.334	698	705	719	rVB	1861686	2967257	2.65%	0.607%
8	7.522	729	737	749	rBV	2308379	3843259	3.43%	0.787%
9	7.881	790	798	809	rBV	4191516	6635943	5.92%	1.358%
10	8.046	810	826	843	rBV2	48454028	108609478	96.87%	22.228%
11	8.345	869	877	885	rBV	2793484	4541305	4.05%	0.929%
12	8.704	930	938	945	rBV	2927913	4621212	4.12%	0.946%
13	9.163	1009	1016	1026	rBV	2209973	3661035	3.27%	0.749%
14	9.734	1105	1113	1120	rBV	125082	217035	0.19%	0.044%
15	9.887	1129	1139	1152	rBV	1825100	3084852	2.75%	0.631%
16	10.422	1222	1230	1237	rBV	2714564	4557192	4.06%	0.933%
17	10.663	1264	1271	1285	rBV2	611708	1278185	1.14%	0.262%
18	10.798	1285	1294	1305	rBV	2504598	4228819	3.77%	0.865%
19	10.945	1310	1319	1330	rBV	2270147	3945096	3.52%	0.807%
20	11.181	1353	1359	1367	rVV	277055	478122	0.43%	0.098%
21	11.551	1415	1422	1434	rBV	164571	308426	0.28%	0.063%
22	12.963	1656	1662	1668	rBV	111487	200093	0.18%	0.041%
23	13.422	1733	1740	1751	rBV2	225559	436847	0.39%	0.089%
24	13.557	1751	1763	1768	rBV	307151	502229	0.45%	0.103%
25	14.039	1835	1845	1853	rBV	4122253	5785185	5.16%	1.184%
26	14.316	1886	1892	1904	rVB	4989480	7525379	6.71%	1.540%
27	14.622	1935	1944	1951	rBV	3212927	4785223	4.27%	0.979%
28	14.822	1971	1978	1991	rBV	2041398	3006630	2.68%	0.615%
29	15.616	2106	2113	2119	rBV	5995869	8499783	7.58%	1.740%
30	15.733	2126	2133	2142	rBV	1649373	2225961	1.99%	0.456%
31	15.945	2164	2169	2181	rVV	107670	172637	0.15%	0.035%
32	16.063	2185	2189	2198	rVB	120282	187003	0.17%	0.038%
33	16.763	2302	2308	2315	rBV2	174785	283274	0.25%	0.058%
34	17.368	2404	2411	2417	rBV	3306894	4826944	4.31%	0.988%
35	17.463	2421	2427	2436	rBV	5653597	8242106	7.35%	1.687%
36	17.751	2468	2476	2483	rBV4	79678	149368	0.13%	0.031%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Title : SVOA CALIBRATION

37	17.868	2492	2496	2501	rBV	93110	124305	0.11%	0.025%
38	18.268	2557	2564	2575	rBV	1250305	1901239	1.70%	0.389%
39	19.192	2717	2721	2727	rVB	187543	232328	0.21%	0.048%
40	19.392	2750	2755	2758	rBV2	113400	174492	0.16%	0.036%
41	19.539	2776	2780	2794	rBV	278868	442585	0.39%	0.091%
42	19.751	2810	2816	2823	rBV	6174575	8292643	7.40%	1.697%
43	20.268	2900	2904	2907	rBV	316246	418105	0.37%	0.086%
44	20.304	2907	2910	2917	rVB	939790	1021143	0.91%	0.209%
45	20.798	2992	2994	2997	rVB	167662	168589	0.15%	0.035%
46	20.833	2997	3000	3003	rBV3	158284	207258	0.18%	0.042%
47	20.956	3016	3021	3025	rBV	1128297	1456320	1.30%	0.298%
48	21.027	3025	3033	3037	rBV	842130	1626133	1.45%	0.333%
49	21.145	3048	3053	3058	rBV	12630414	15283409	13.63%	3.128%
50	21.192	3058	3061	3068	rVV4	590916	1267526	1.13%	0.259%
51	21.262	3068	3073	3075	rVV	4923190	7408262	6.61%	1.516%
52	21.286	3075	3077	3083	rVB	8720209	9718482	8.67%	1.989%
53	21.445	3093	3104	3109	rBV3	940636	2811035	2.51%	0.575%
54	21.498	3110	3113	3116	rVV2	972862	1360623	1.21%	0.278%
55	21.539	3116	3120	3131	rVB2	3786303	5362572	4.78%	1.097%
56	21.715	3146	3150	3154	rBV	356004	468181	0.42%	0.096%
57	22.198	3225	3232	3243	rBV2	4823582	8001266	7.14%	1.638%
58	22.827	3335	3339	3346	rVB	601606	905106	0.81%	0.185%
59	23.262	3407	3413	3416	rBV	2472115	3949259	3.52%	0.808%
60	23.303	3416	3420	3432	rVV	3419281	6250417	5.57%	1.279%
61	23.409	3434	3438	3453	rVB	345088	689235	0.61%	0.141%
62	23.809	3499	3506	3516	rVB2	3893121	7978231	7.12%	1.633%
63	23.968	3526	3533	3539	rBV	2323946	4472850	3.99%	0.915%
64	24.503	3619	3624	3632	rVB	480166	1025880	0.91%	0.210%
65	24.650	3644	3649	3657	rVB	818781	1749428	1.56%	0.358%
66	24.744	3658	3665	3676	rBV	1962604	4747607	4.23%	0.972%
67	24.874	3682	3687	3700	rVB5	759227	2320867	2.07%	0.475%
68	25.415	3774	3779	3789	rVB	669949	1652785	1.47%	0.338%
69	26.003	3871	3879	3893	rVB7	878463	2717476	2.42%	0.556%
70	26.709	3993	3999	4016	rVB2	620250	2031799	1.81%	0.416%
71	27.656	4150	4160	4175	rVB2	1823401	6239234	5.56%	1.277%
72	28.515	4291	4306	4327	rVB2	11355061	44947759	40.09%	9.199%
73	28.915	4362	4374	4398	rVB6	2325191	10311477	9.20%	2.110%

Sum of corrected areas: 488617400

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Acq On : 18 Dec 2023 21:10
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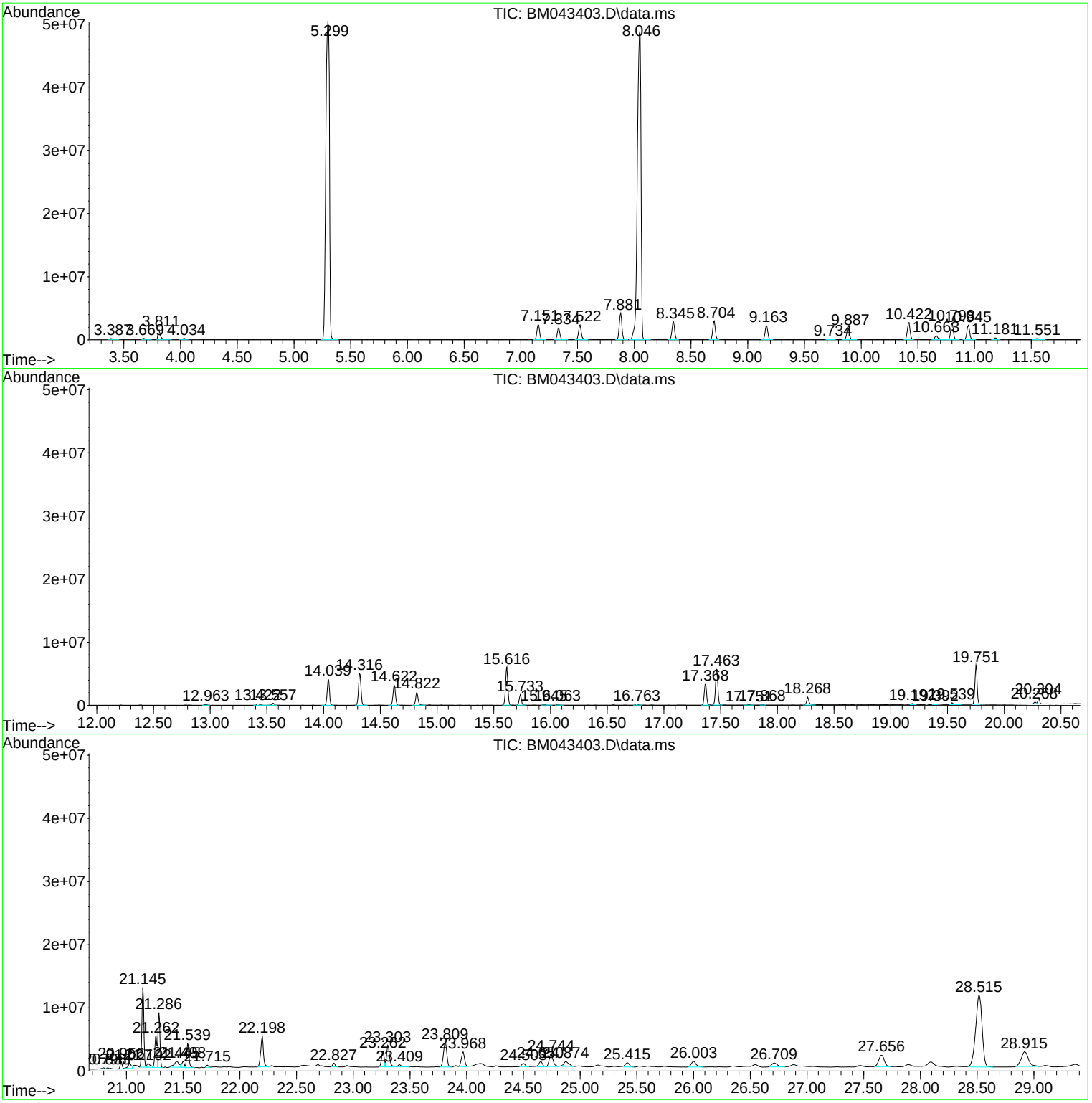
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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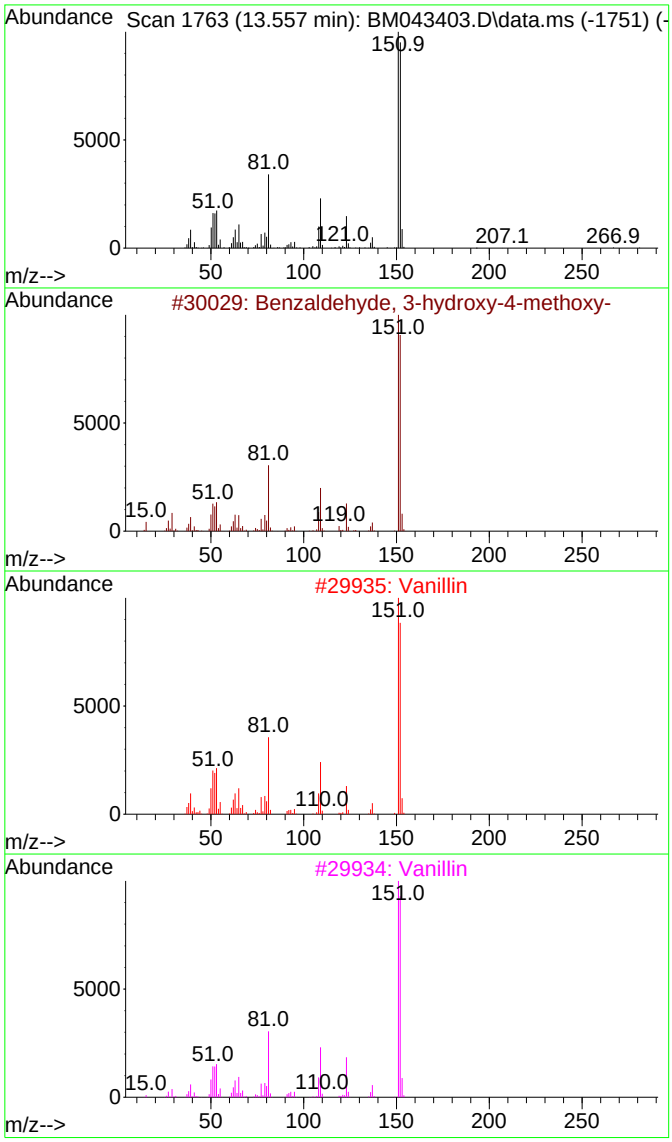
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

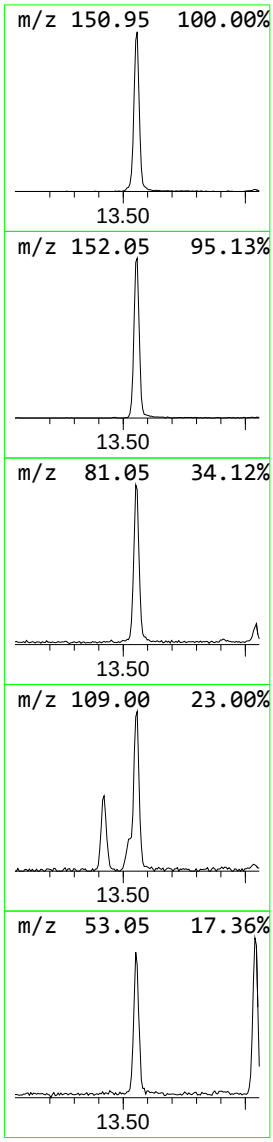
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzaldehyde, 3-hydroxy-4-m... Concentration Rank 28

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.557	2.10 ng/ul	502229	Acenaphthene-d10	14.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
2	Vanillin	152	C8H8O3	000121-33-5	97
3	Vanillin	152	C8H8O3	000121-33-5	97
4	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
5	Vanillin	152	C8H8O3	000121-33-5	96





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

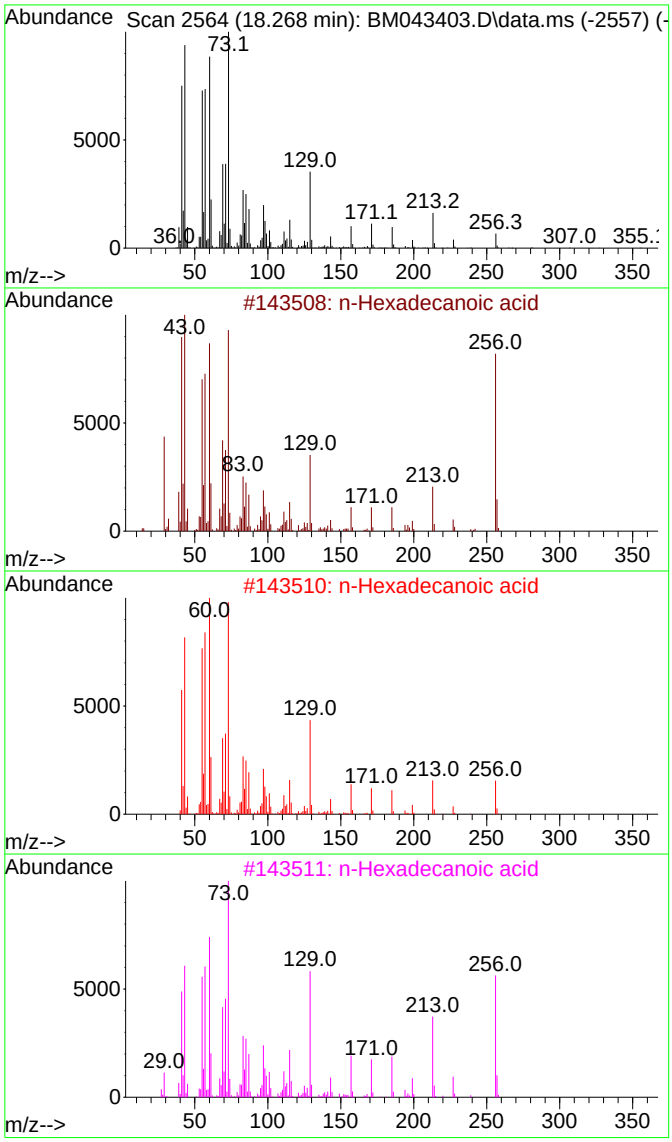
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

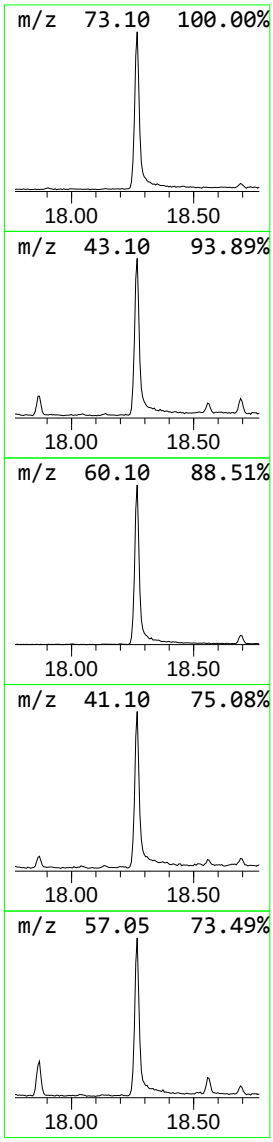
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 n-Hexadecanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.268	7.88 ng/ul	1901240	Phenanthrene-d10	17.368

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

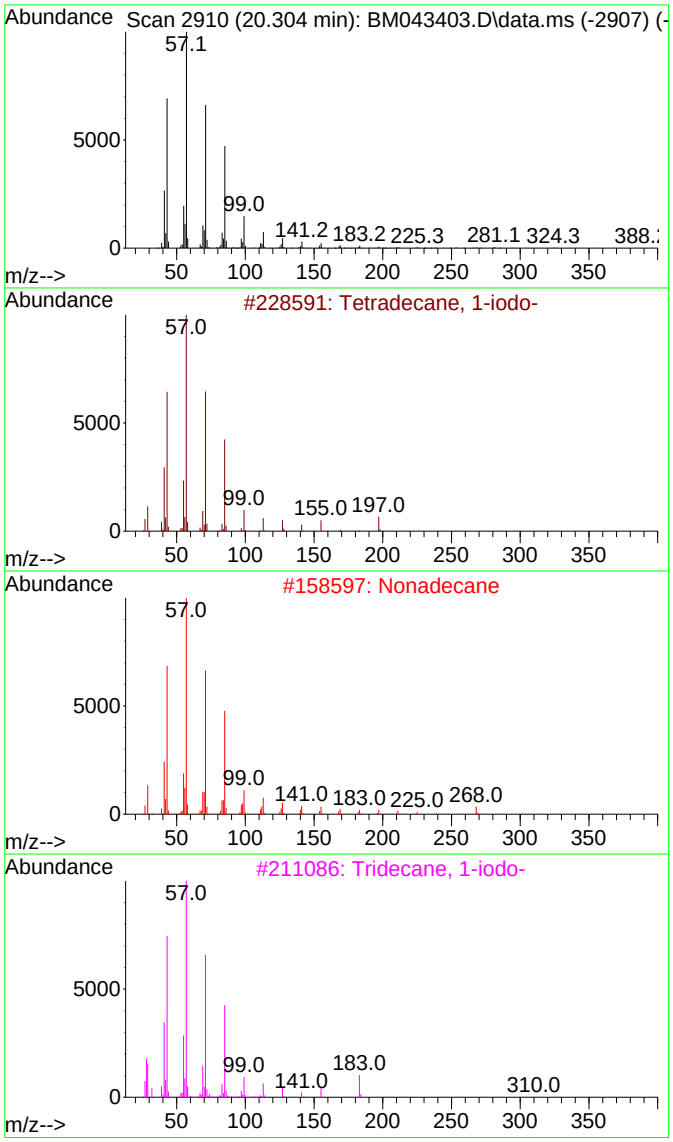
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

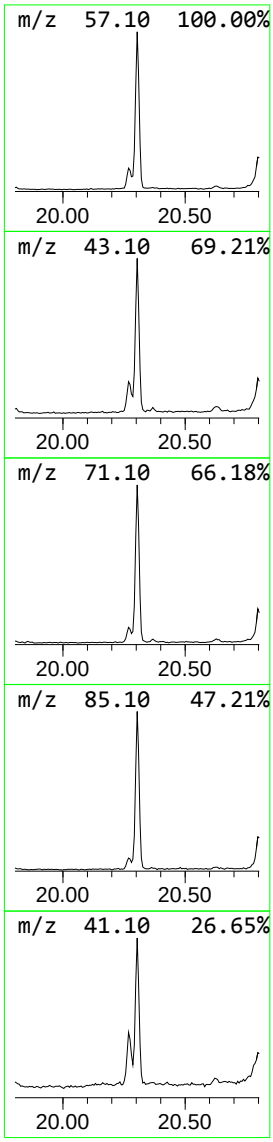
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Tetradecane, 1-iodo- Concentration Rank 25

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.304	3.81 ng/ul	1021140	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	91
2	Nonadecane	268	C19H40	000629-92-5	90
3	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5	Heneicosane	296	C21H44	000629-94-7	83





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Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
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Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

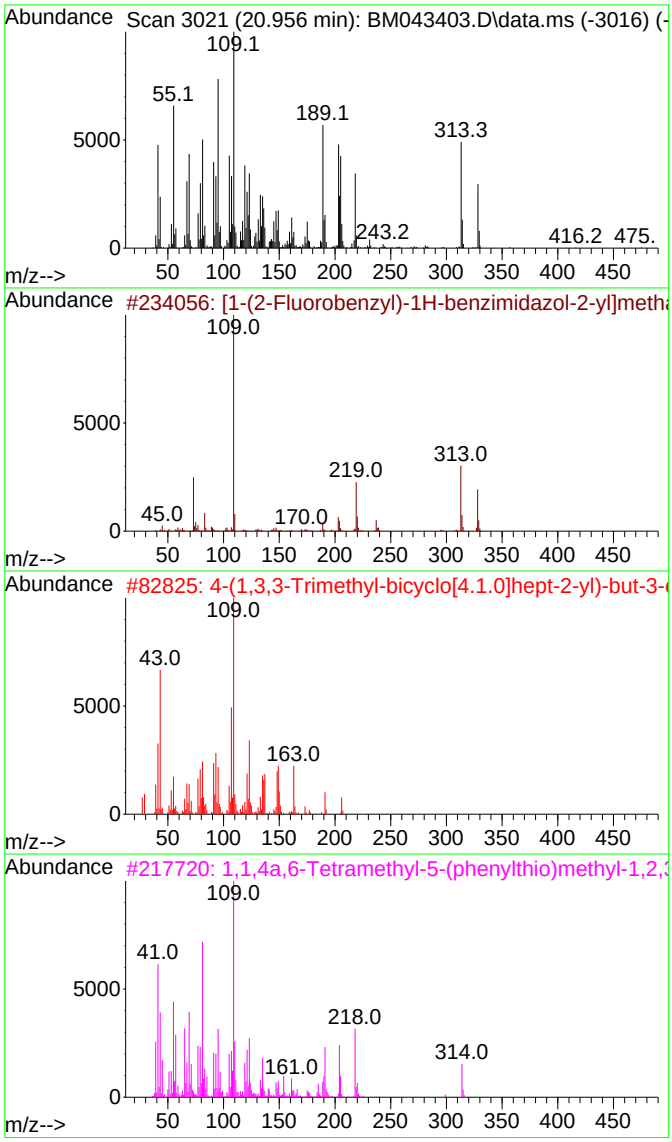
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

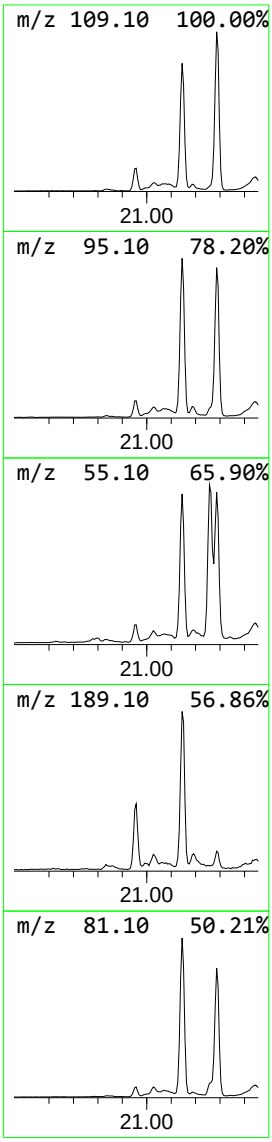
****

Peak Number 7 unknown-01 Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.956	5.43 ng/ul	1456320	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1-(2-Fluorobenzyl)-1H-benzimida...	328	C18H21FN2OSi	1010474-87-2	27
2	4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	25
3	1,1,4a,6-Tetramethyl-5-(phenylth...	314	C21H30S	155191-62-1	25
4	4-(3,5-Dimethylpyrazol-1-yl)-1,2...	189	C8H7N5O	1000436-50-1	20
5	2-Caren-4-ol	152	C10H16O	006617-35-2	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043403.D
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Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

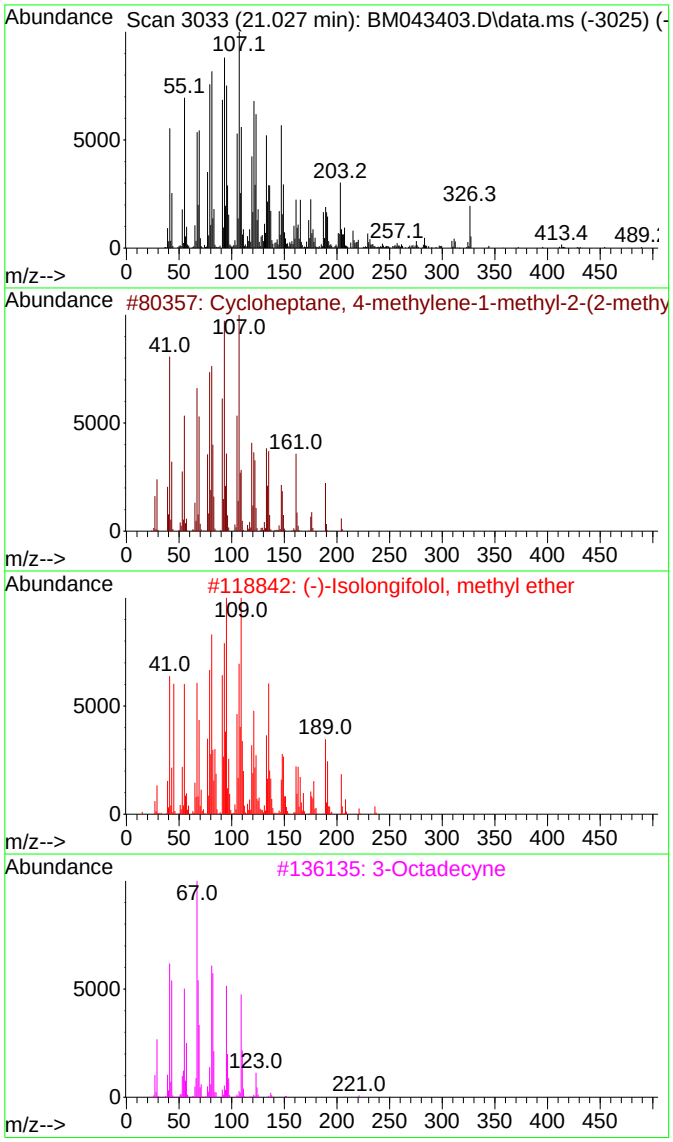
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

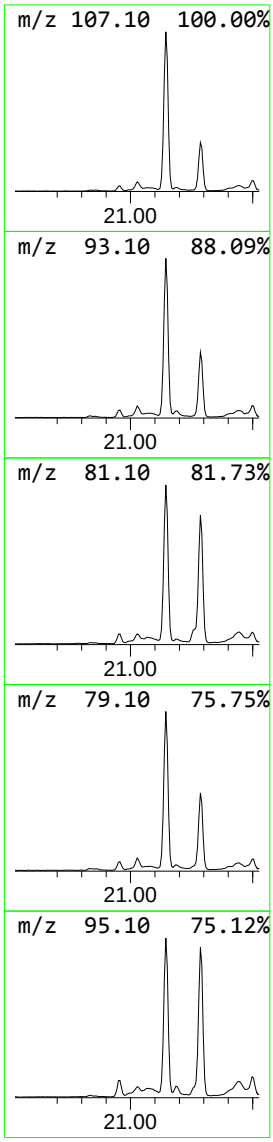
****

Peak Number 8 unknown-02 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.027	6.06 ng/ul	1626130	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptane, 4-methylene-1-meth...	204	C15H24	1010159-38-5	46
2	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	38
3	3-Octadecyne	250	C18H34	061886-64-4	30
4	(2R,3R,4aR,5S,8aS)-2-Hydroxy-4a,...	234	C15H22O2	005090-89-1	30
5	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

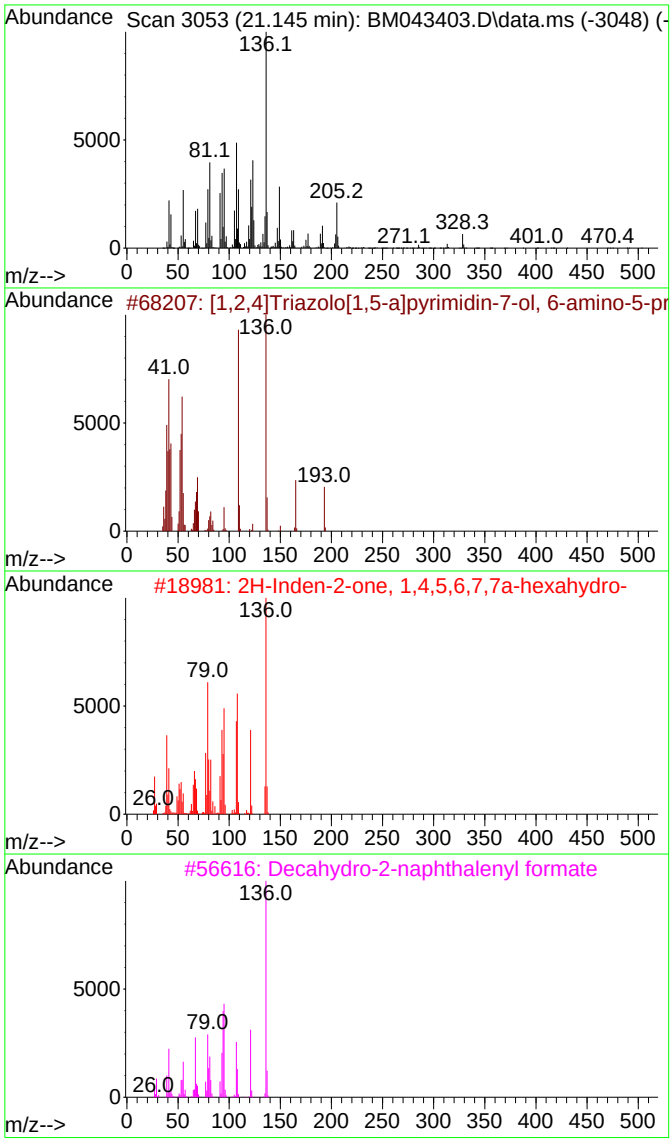
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

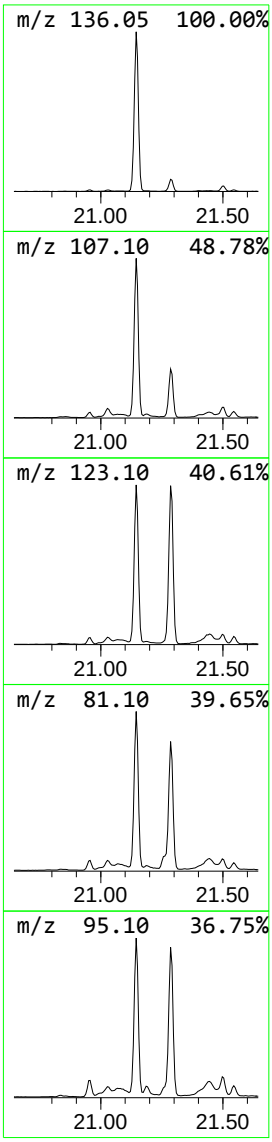
****

Peak Number 9 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.145	57.00 ng/ul	15283400	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1,2,4]Triazolo[1,5-a]pyrimidin-...	193	C8H11N5O	1000362-66-7	38
2	2H-Inden-2-one, 1,4,5,6,7,7a-hex...	136	C9H12O	039163-29-6	35
3	Decahydro-2-naphthalenyl formate	182	C11H18O2	010519-12-7	35
4	3H-Cyclopenta[c]pyridazin-3-one,...	136	C7H8N2O	1000338-22-1	35
5	Benzaldehyde, 3-methoxy-	136	C8H8O2	000591-31-1	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

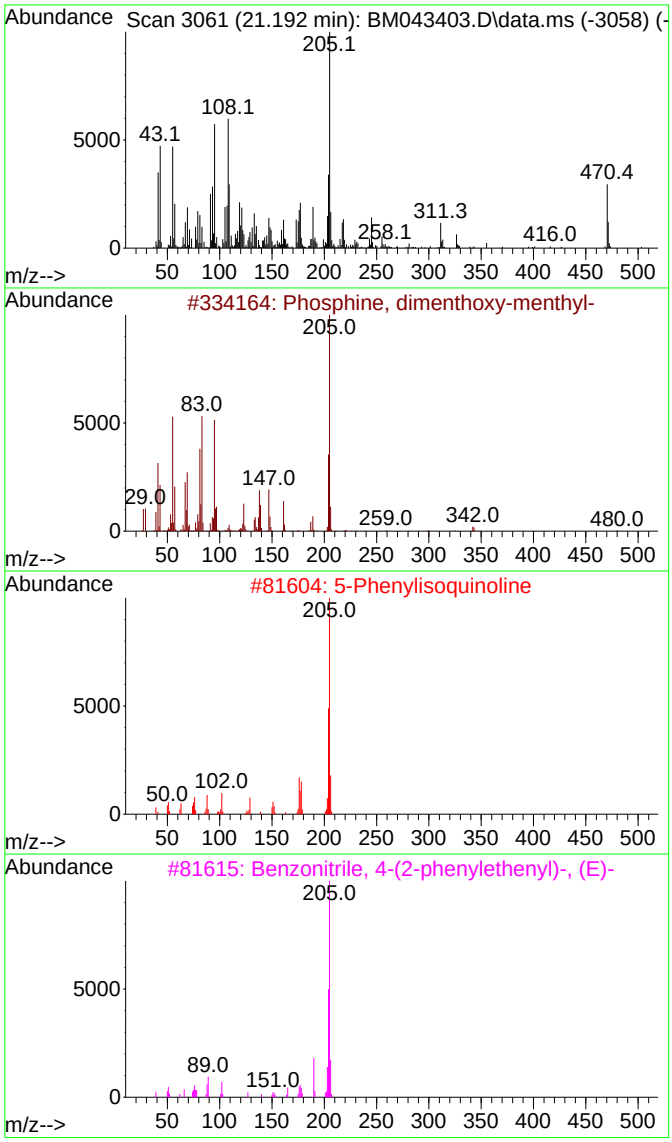
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

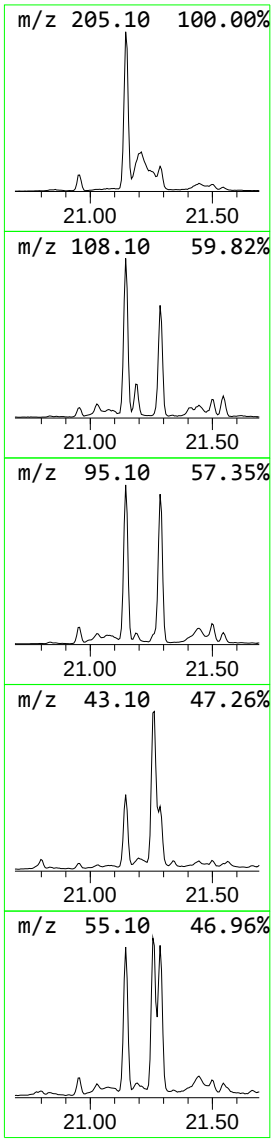
****

Peak Number 10 unknown-04 Concentration Rank 22

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.192	4.73 ng/ul	1267530	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphine, dimenthoxy-menthyl-	480	C30H57O2P	123973-40-0	47
2	5-Phenylisoquinoline	205	C15H11N	024464-35-5	30
3	Benzonitrile, 4-(2-phenylethenyl...	205	C15H11N	013041-79-7	27
4	5-(1H-Pyrrol-3-ylmethylene)-pyri...	205	C9H7N3O3	1000318-16-3	27
5	Quinoline, 2-phenyl-	205	C15H11N	000612-96-4	25





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Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

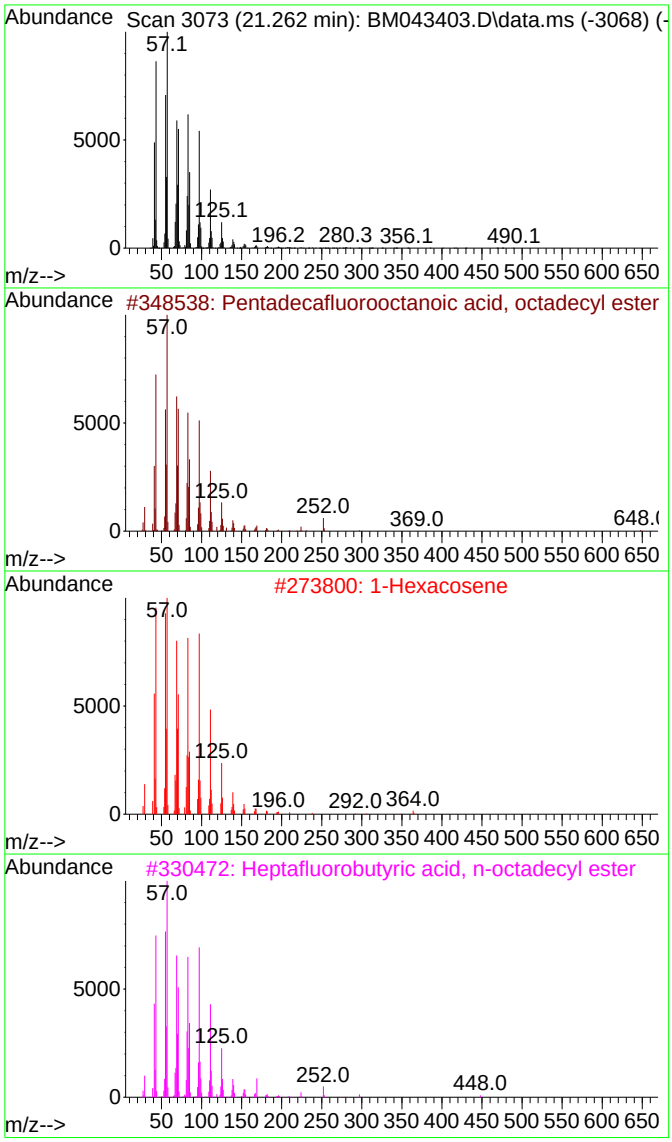
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

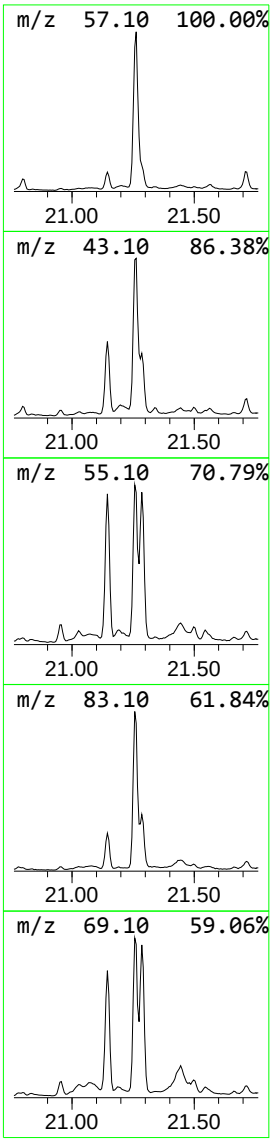
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Pentadecafluorooctanoic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.262	27.63 ng/ul	7408260	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	1-Hexacosene	364	C26H52	018835-33-1	93
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91





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Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

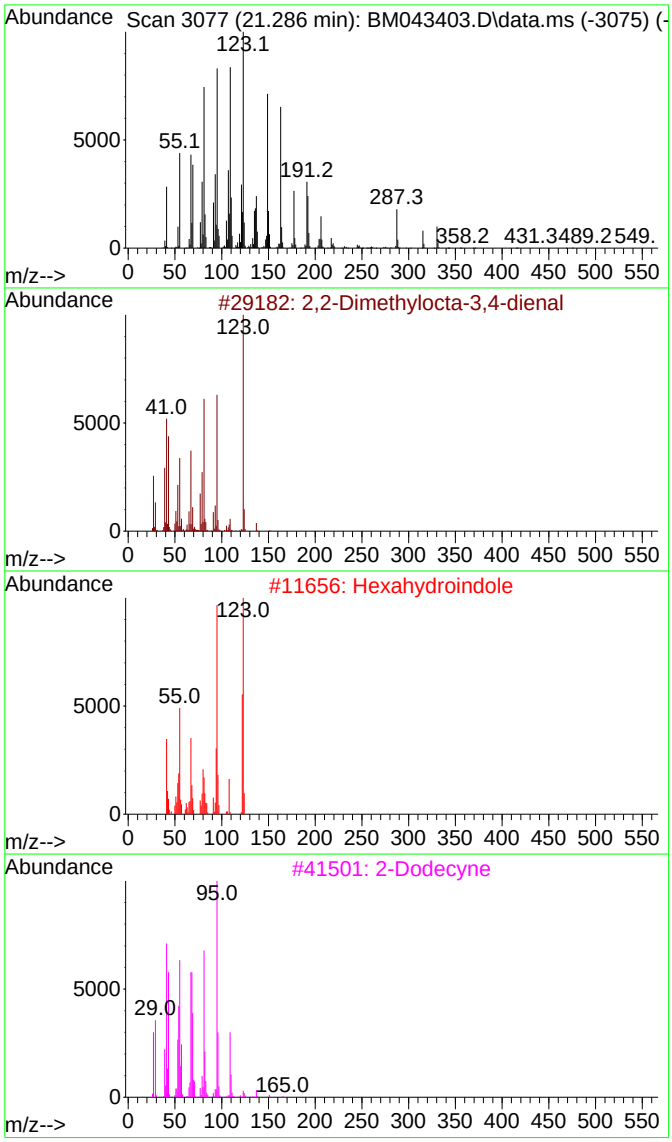
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

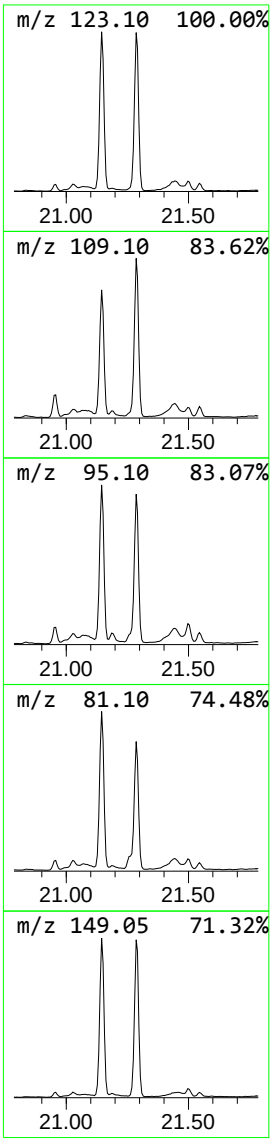
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 unknown-05 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.286	36.25 ng/ul	9718480	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylocta-3,4-dienal	152	C10H16O	000590-71-6	49
2	Hexahydroindole	123	C8H13N	018159-32-5	30
3	2-Dodecyne	166	C12H22	000629-49-2	30
4	1H-Indene, 5-decyloctahydro-	264	C19H36	055044-35-4	27
5	Phthalic acid, 4-fluorobenzyl pr...	316	C18H17FO4	1010377-74-1	25





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Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

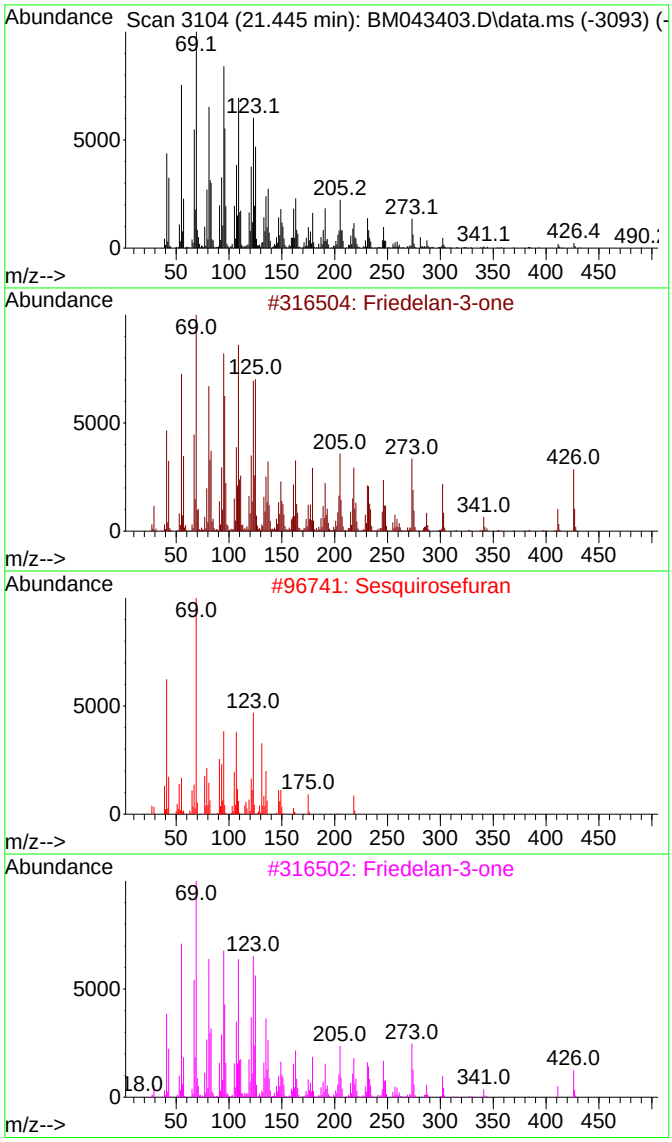
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

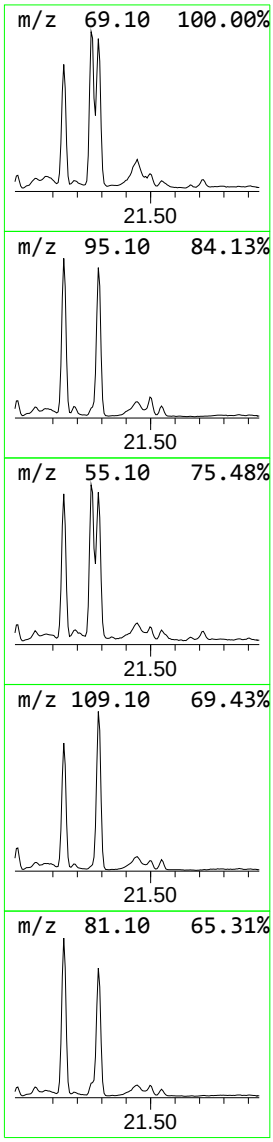
****

Peak Number 13 Sesquirosefuran Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.445	10.48 ng/ul	2811040	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Friedelan-3-one	426	C30H50O	000559-74-0	98
2	Sesquirosefuran	218	C15H22O	039007-93-7	95
3	Friedelan-3-one	426	C30H50O	000559-74-0	91
4	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	53
5	Cedrol	222	C15H26O	000077-53-2	46





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Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

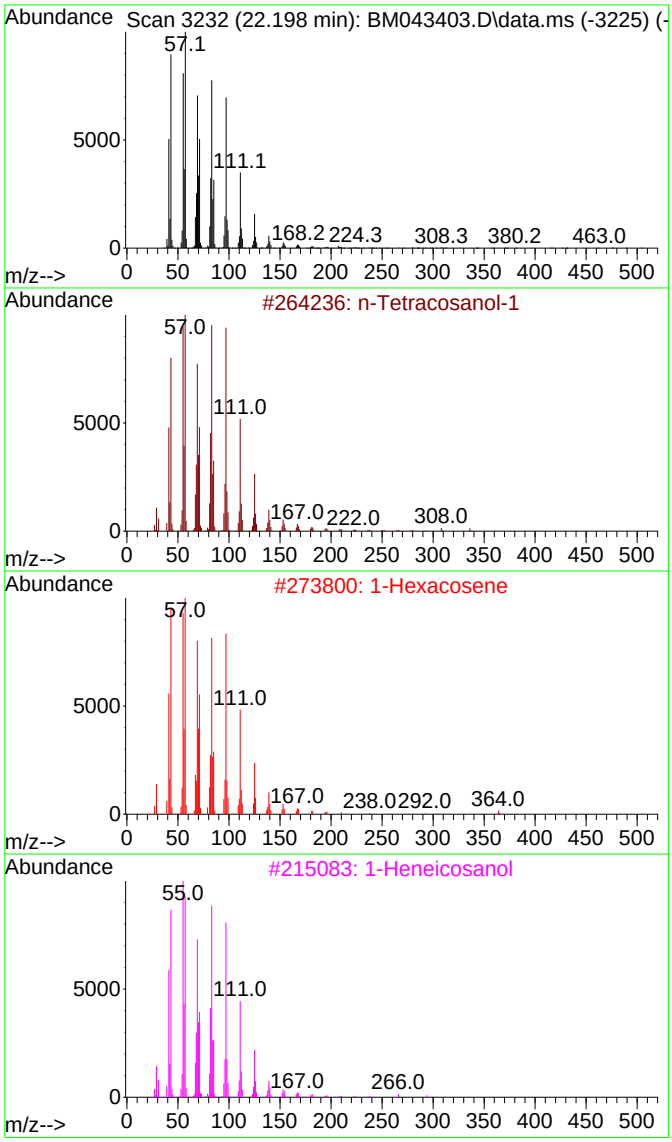
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

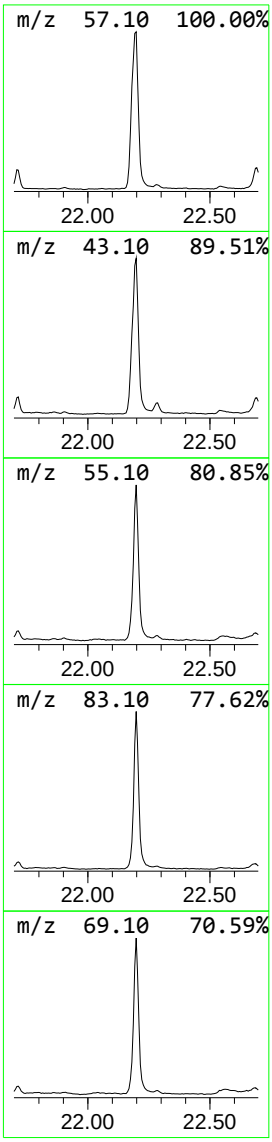
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.198	29.84 ng/ul	8001270	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	1-Hexacosene	364	C26H52	018835-33-1	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	93
4	1-Docosene	308	C22H44	001599-67-3	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	91





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Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

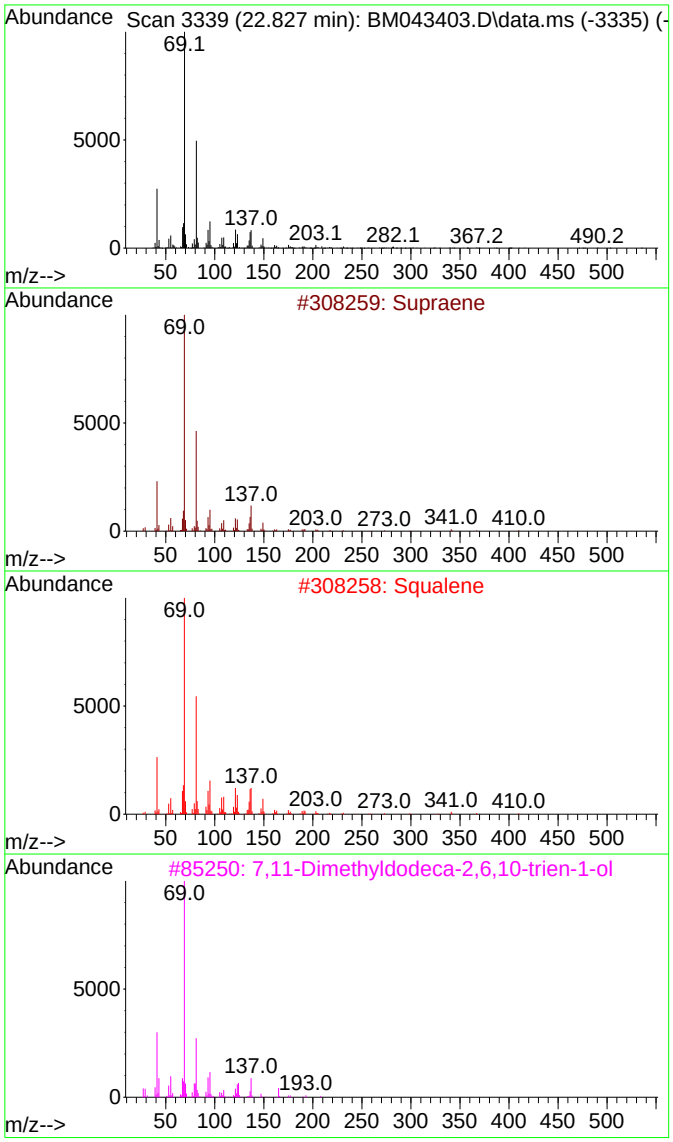
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

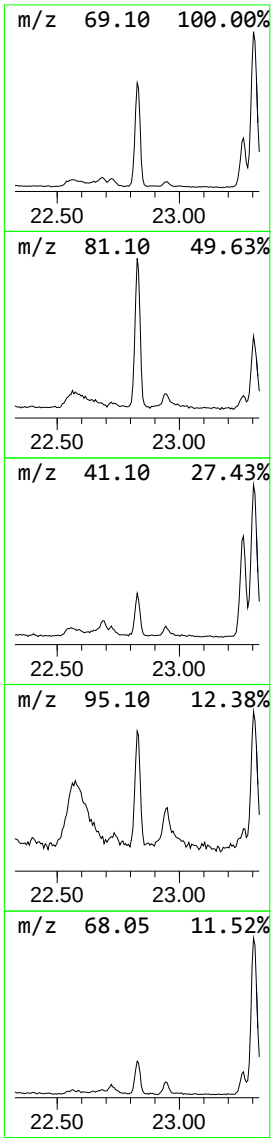
****

Peak Number 15 Supraene Concentration Rank 24

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.827	4.05 ng/ul	905106	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	90
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	64
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	64





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Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

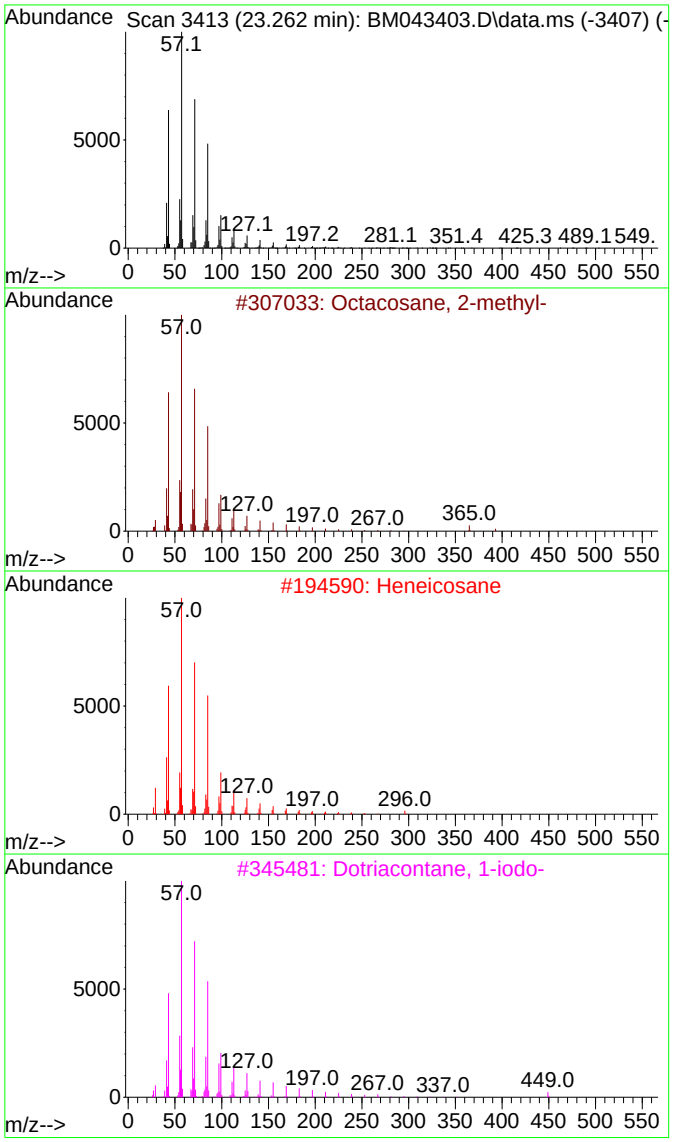
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

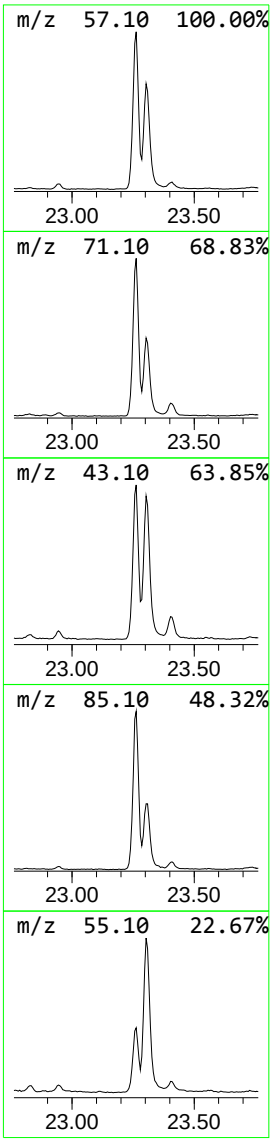
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.262	17.66 ng/ul	3949260	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Hexadecane	226	C16H34	000544-76-3	87





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Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

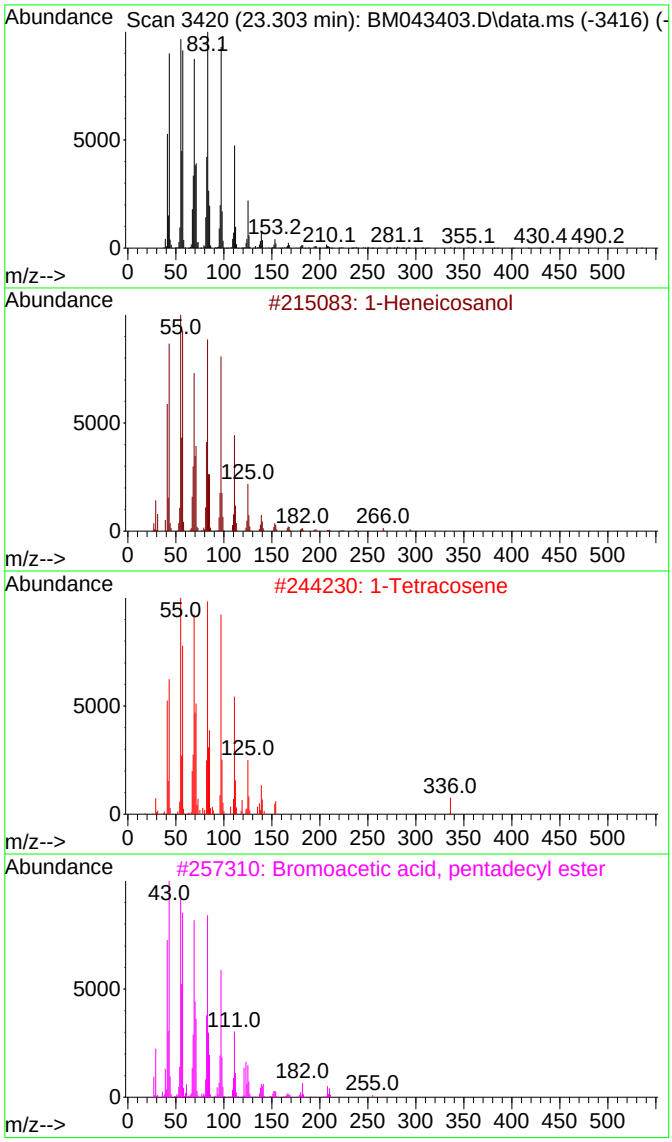
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

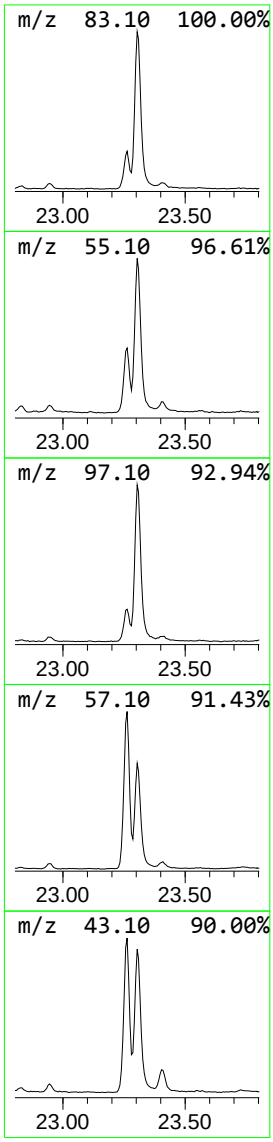
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.303	27.95 ng/ul	6250420	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	1-Tetracosene	336	C24H48	010192-32-2	89
3	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	87
4	1-Heptacosanol	396	C27H56O	002004-39-9	83
5	1-Octadecanol	270	C18H38O	000112-92-5	81





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Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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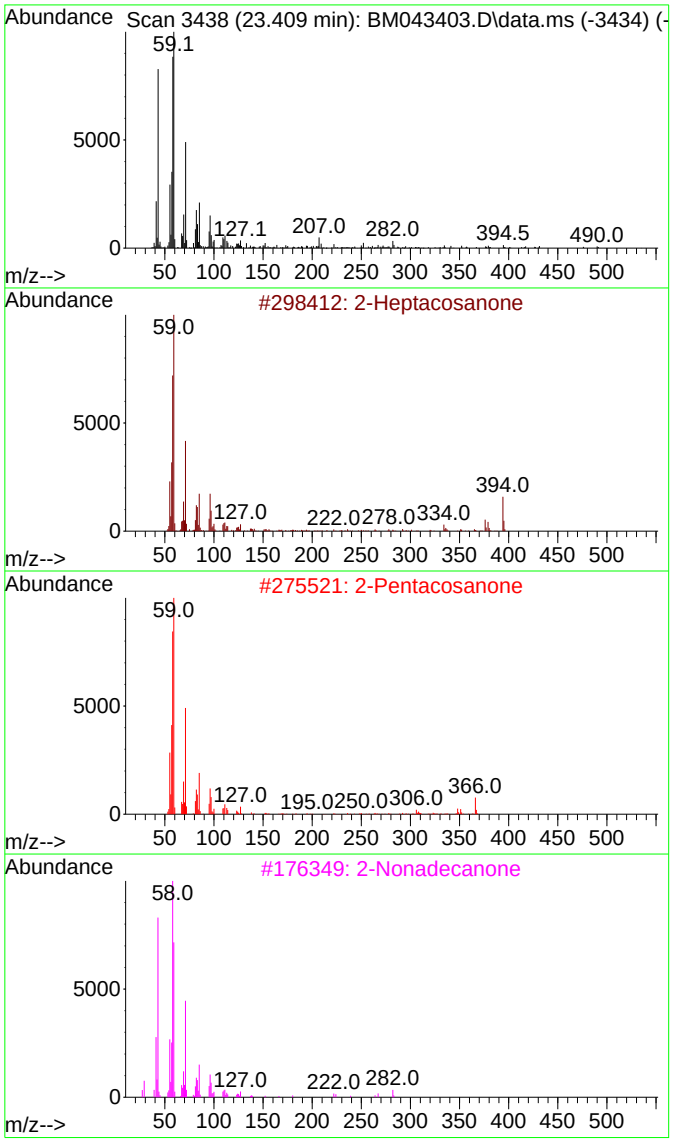
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

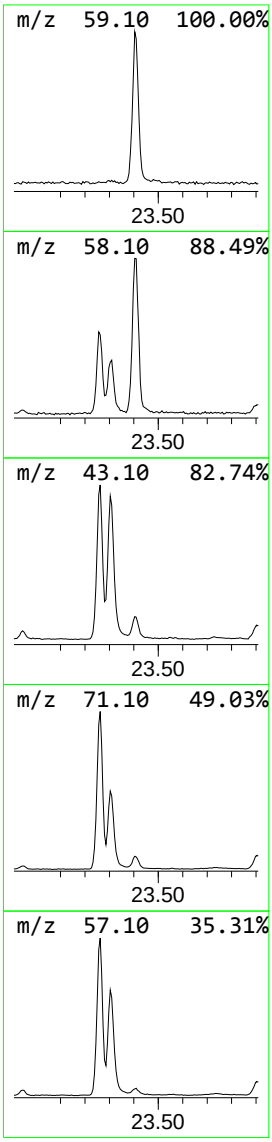
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 18 2-Heptacosanone Concentration Rank 26

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.409	3.08 ng/ul	689235	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptacosanone	394	C27H54O	007796-19-2	93
2	2-Pentacosanone	366	C25H50O	075207-54-4	90
3	2-Nonadecanone	282	C19H38O	000629-66-3	89
4	2-Nonadecanone	282	C19H38O	000629-66-3	64
5	2-Nonadecanone	282	C19H38O	000629-66-3	62





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Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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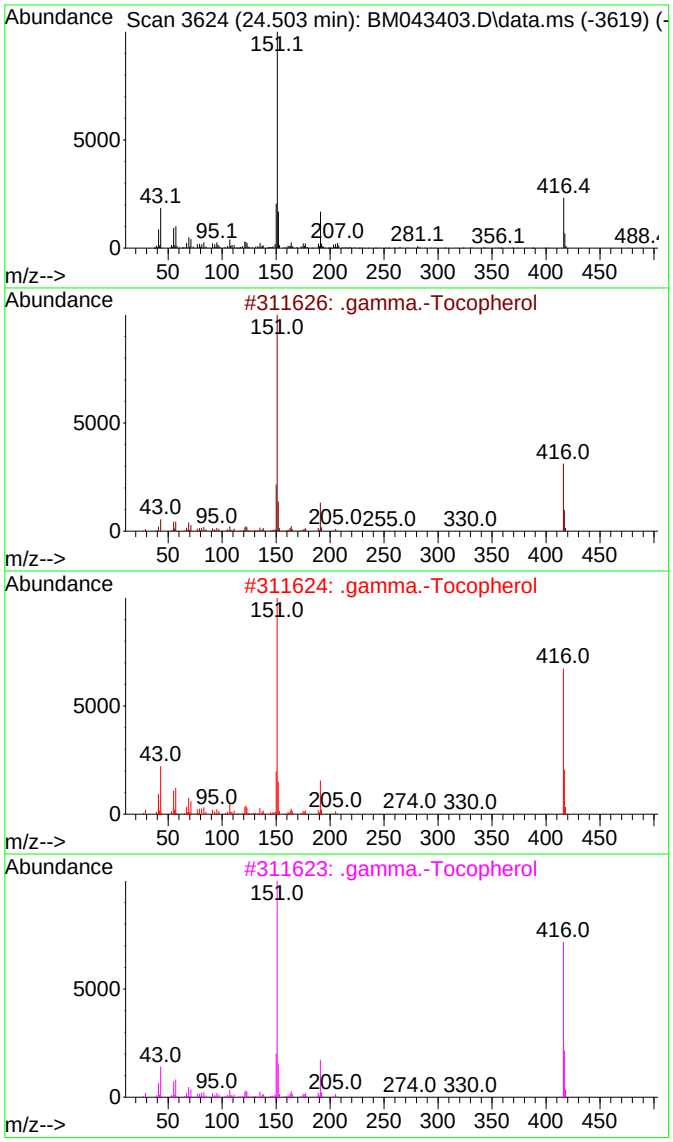
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

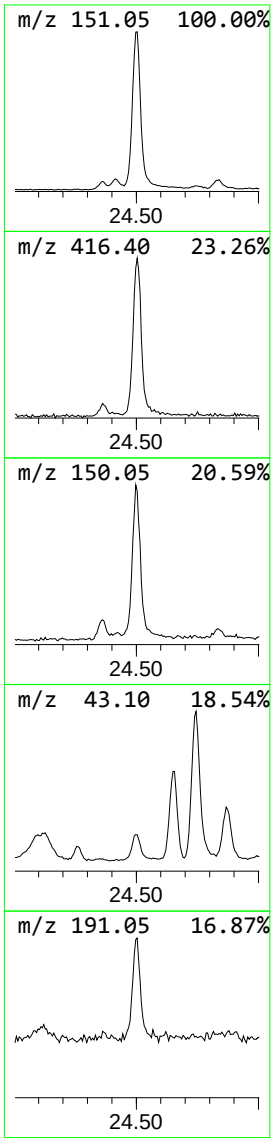
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 .gamma.-Tocopherol Concentration Rank 23

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.503	4.59 ng/ul	1025880	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Tocopherol	416	C28H48O2	007616-22-0	97
2	.gamma.-Tocopherol	416	C28H48O2	007616-22-0	95
3	.gamma.-Tocopherol	416	C28H48O2	007616-22-0	95
4	.gamma.-Tocopherol	416	C28H48O2	007616-22-0	93
5	3,4-Dihydro-3,5,8-trimethyl-3-(4...	458	C30H50O3	1000105-71-9	64





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Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0AX5

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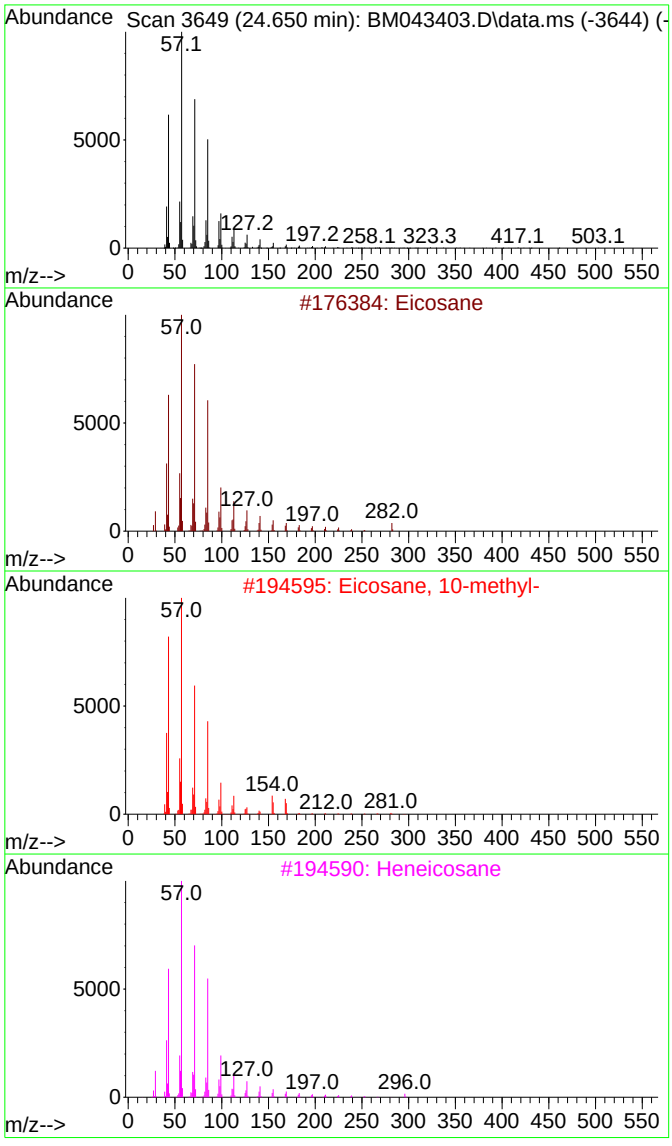
Quant Title : SVOA CALIBRATION

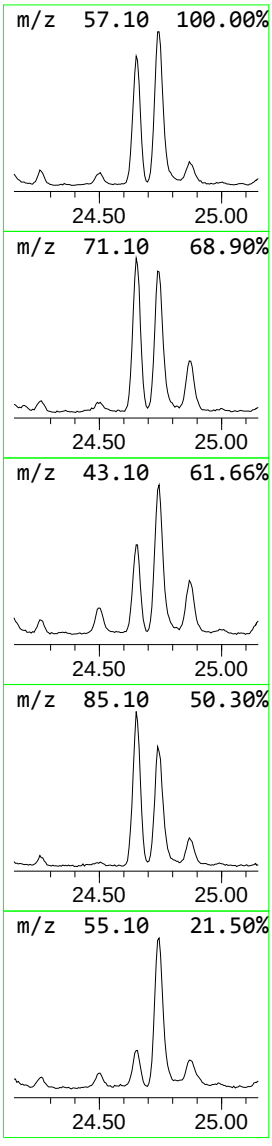
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 (DEL) Alkane: Straight-Chai... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.650	7.82 ng/ul	1749430	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	90
5	Hexatriacontane	507	C36H74	000630-06-8	90





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Sample : 05807-03
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0AX5

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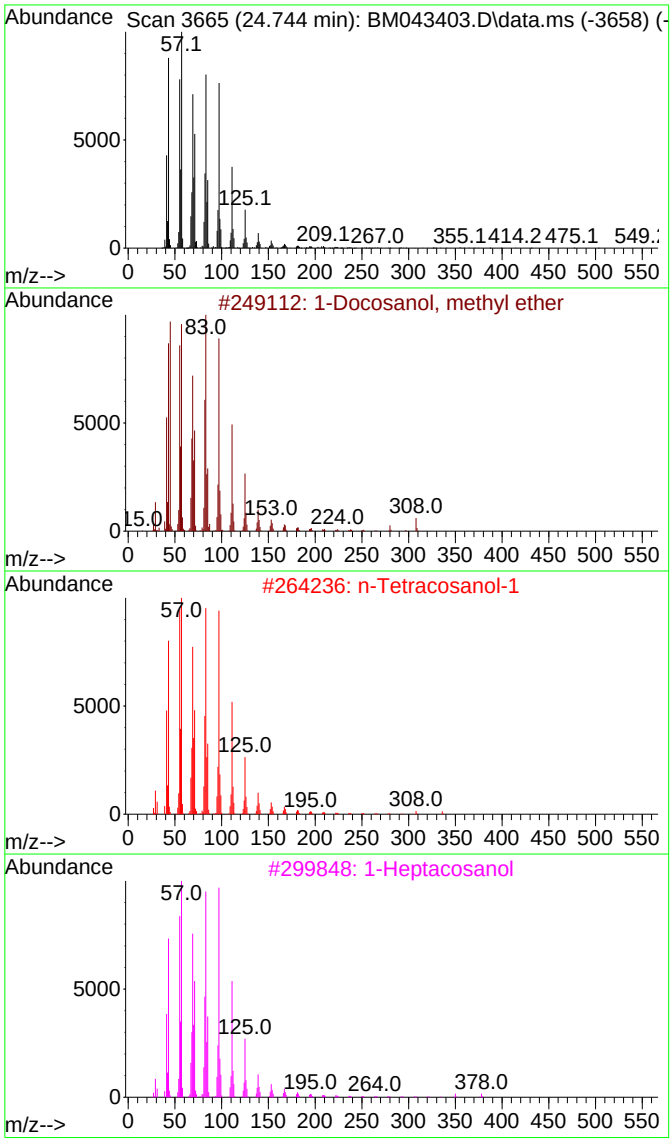
Quant Title : SVOA CALIBRATION

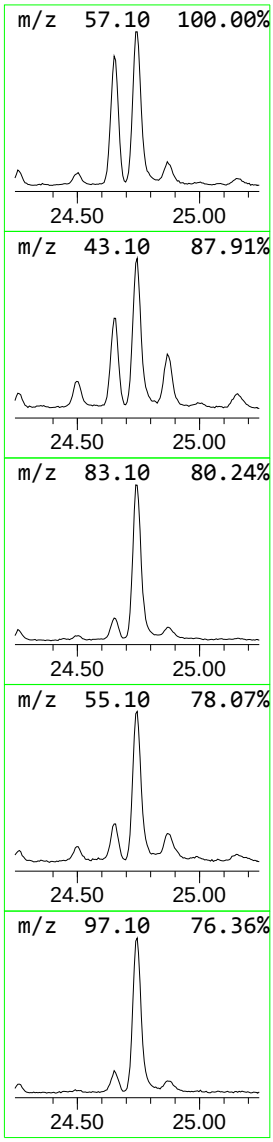
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 21 1-Docosanol, methyl ether Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.744	21.23 ng/ul	4747610	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
5	Behenic alcohol	326	C22H46O	000661-19-8	93





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Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

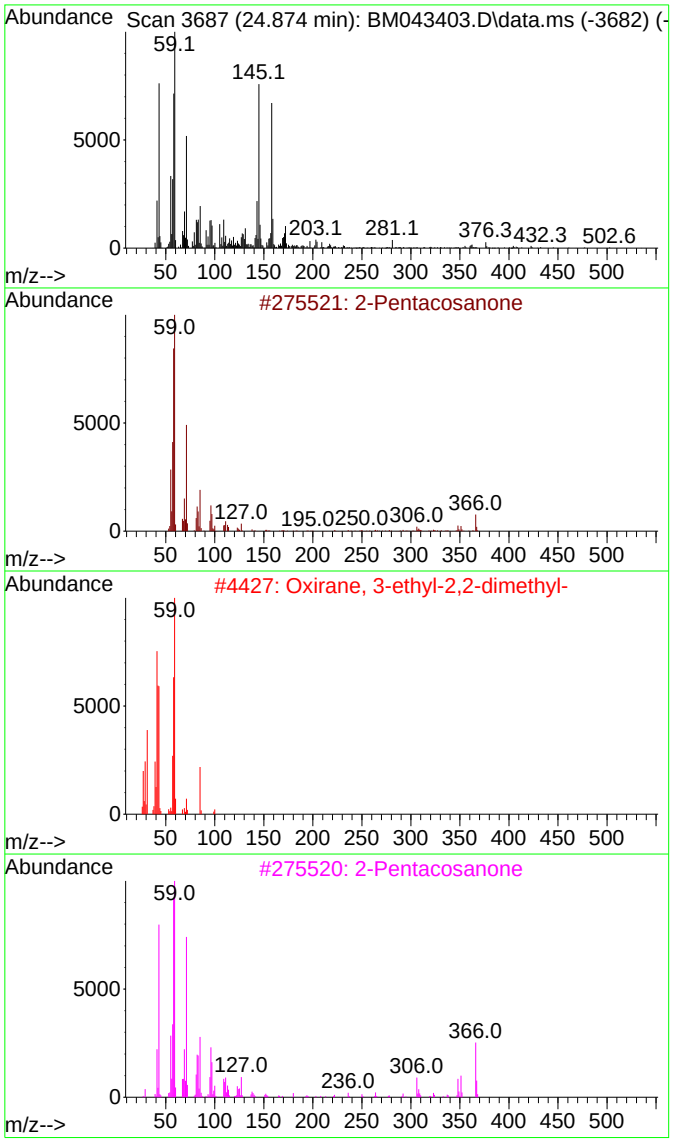
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

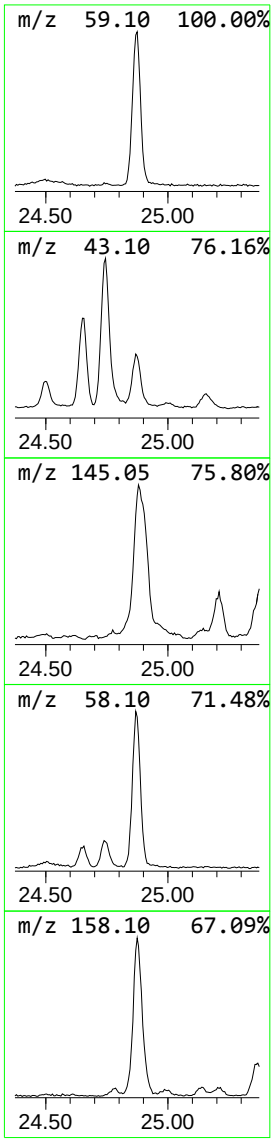
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 22 unknown-06 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.874	10.38 ng/ul	2320870	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentacosanone	366	C25H50O	075207-54-4	43
2	Oxirane, 3-ethyl-2,2-dimethyl-	100	C6H12O	001192-22-9	27
3	2-Pentacosanone	366	C25H50O	075207-54-4	27
4	1,3,4-thiadiazole-2,5-diamine, N...	158	C5H10N4S	1000404-35-9	25
5	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

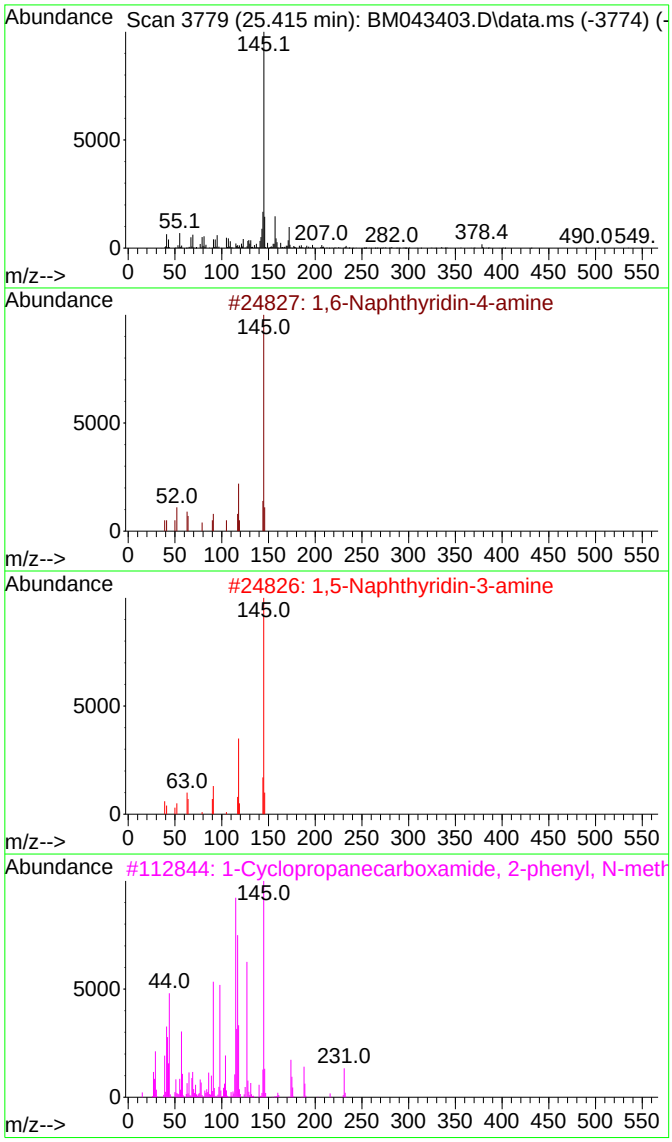
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

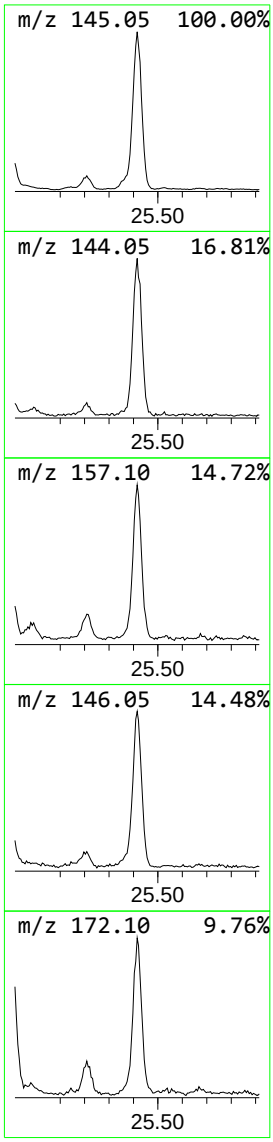
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 23 1,6-Naphthyridin-4-amine Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.415	7.39 ng/ul	1652790	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Naphthyridin-4-amine	145	C8H7N3	028593-08-0	64
2	1,5-Naphthyridin-3-amine	145	C8H7N3	014756-77-5	59
3	1-Cyclopropanecarboxamide, 2-phe...	231	C15H21NO	1000437-34-6	59
4	2,3,6-Trifluorobenzyl alcohol, 3...	232	C12H15F3O	1000375-26-3	52
5	1H-Indole, 2,5-dimethyl-	145	C10H11N	001196-79-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

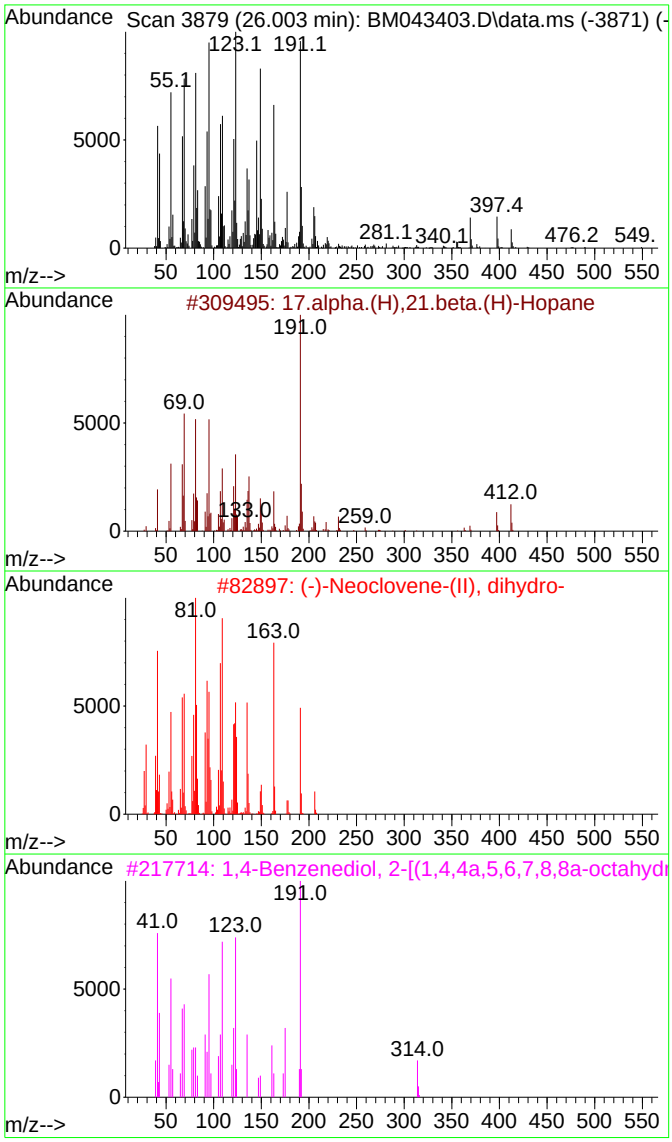
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

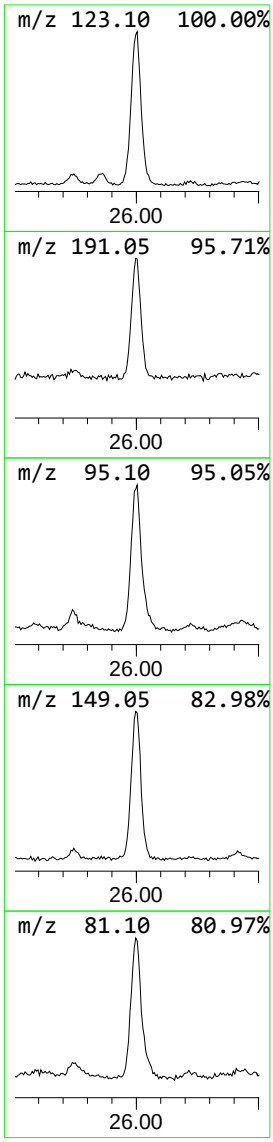
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 24 unknown-07 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.003	12.15 ng/ul	2717480	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	43
2	(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	43
3	1,4-Benzenediol, 2-[(1,4,4a,5,6,...	314	C21H30O2	039707-55-6	38
4	Thioctic acid	206	C8H14O2S2	001077-28-7	27
5	Hexahydroindole	123	C8H13N	018159-32-5	18





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Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

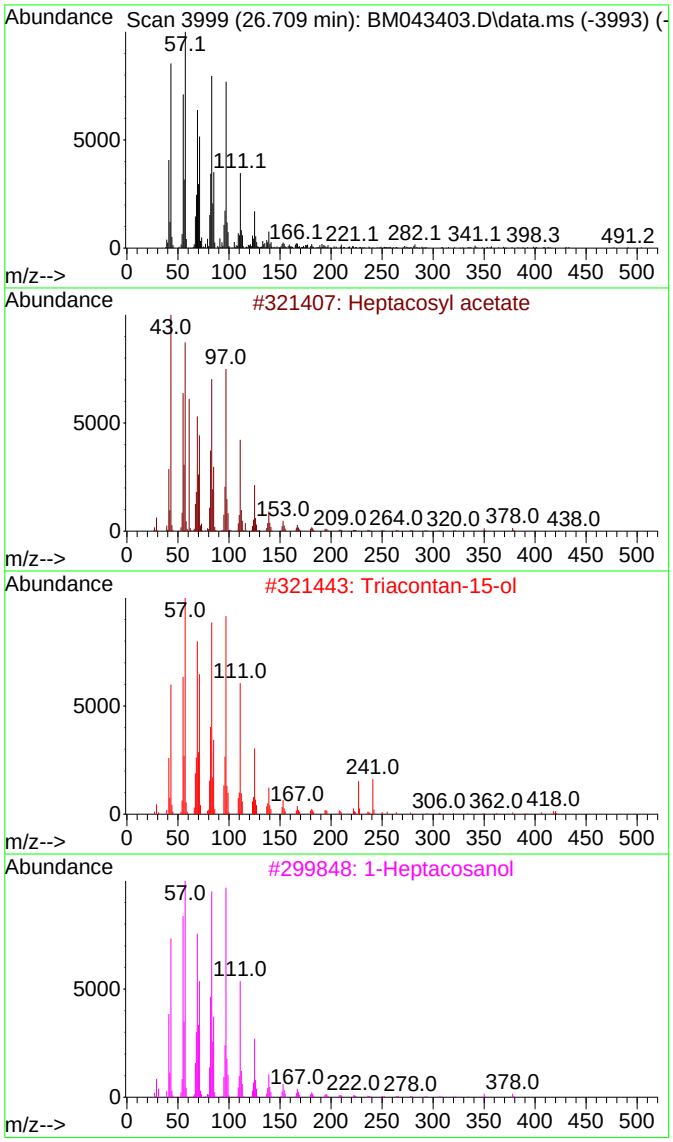
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

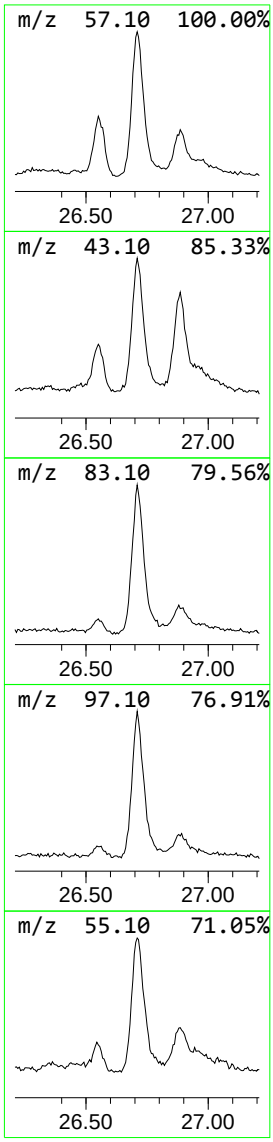
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 25 Heptacosyl acetate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.709	9.09 ng/ul	2031800	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosyl acetate	438	C29H58O2	1000351-78-2	94
2	Triacontan-15-ol	438	C30H62O	031849-26-0	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	93
4	Octacosanol	410	C28H58O	000557-61-9	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	91





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Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

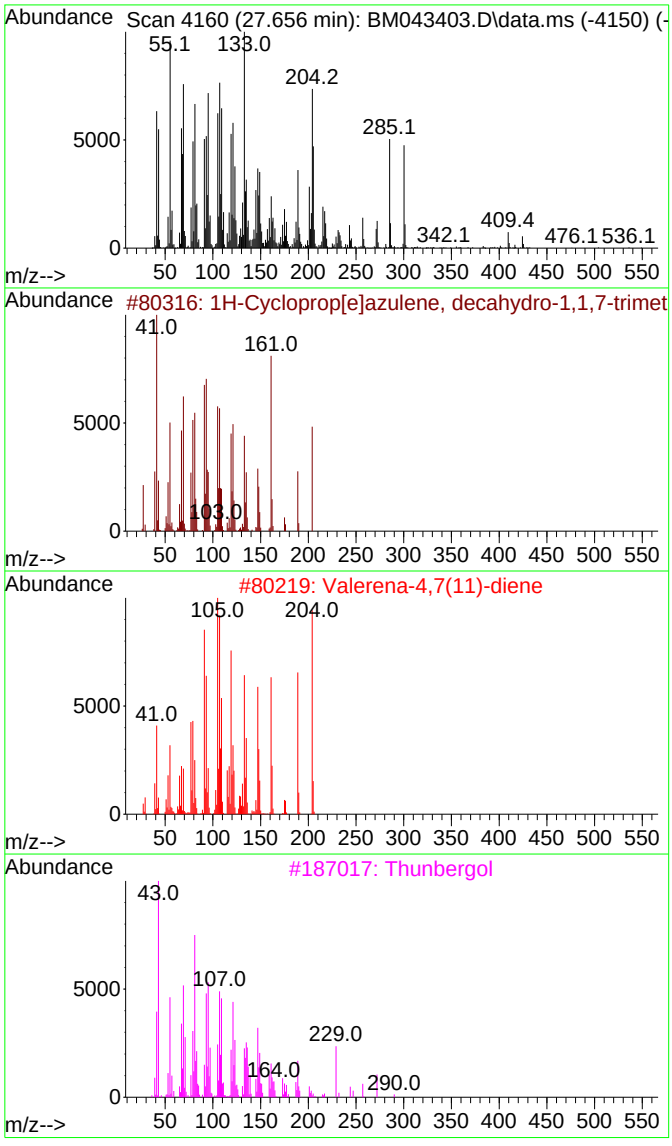
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

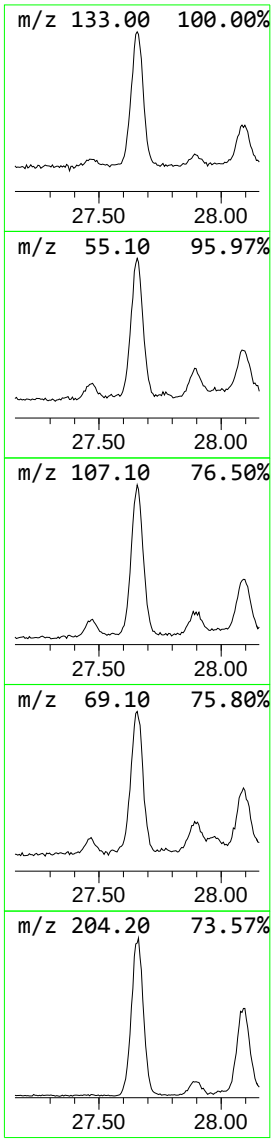
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 26 1H-Cycloprop[e]azulene, dec... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.656	27.90 ng/ul	6239230	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cycloprop[e]azulene, decahydr...	204	C15H24	072747-25-2	64
2	Valerena-4,7(11)-diene	204	C15H24	351222-66-7	52
3	Thunbergol	290	C20H34O	025269-17-4	47
4	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	43
5	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	43





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Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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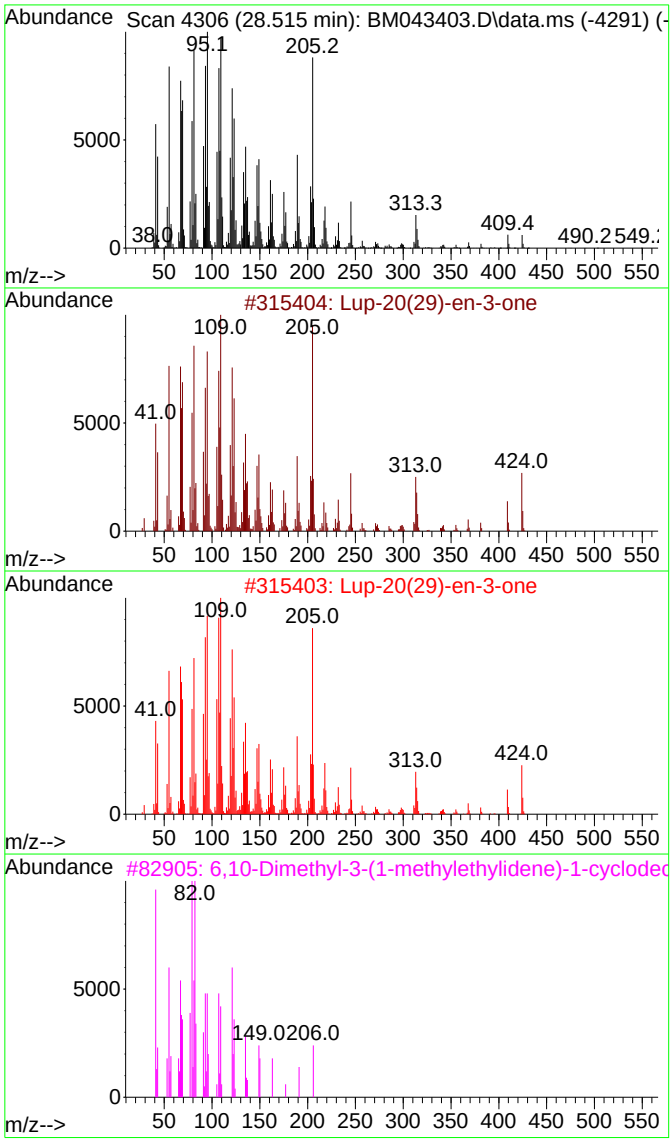
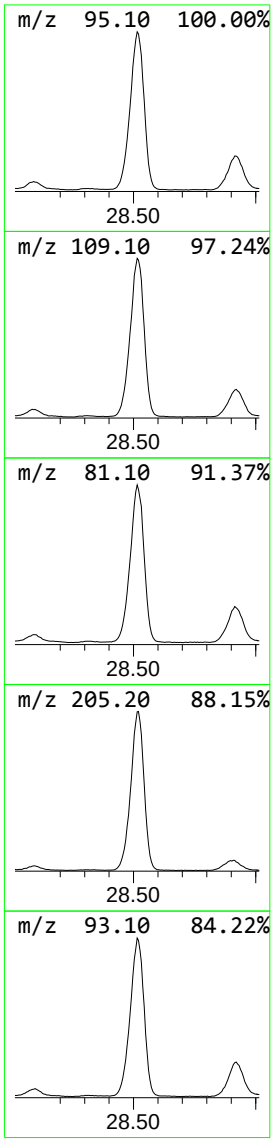
Peak Number 27 Lup-20(29)-en-3-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.515	200.98 ng/ul	44947800	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
2	Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
3	6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	60
4	1-Isopropenyl-3-propenylcyclopen...	150	C11H18	1000192-81-2	48
5	Guaia-9,11-diene	204	C15H24	1000374-19-8	45





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Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
C0AX5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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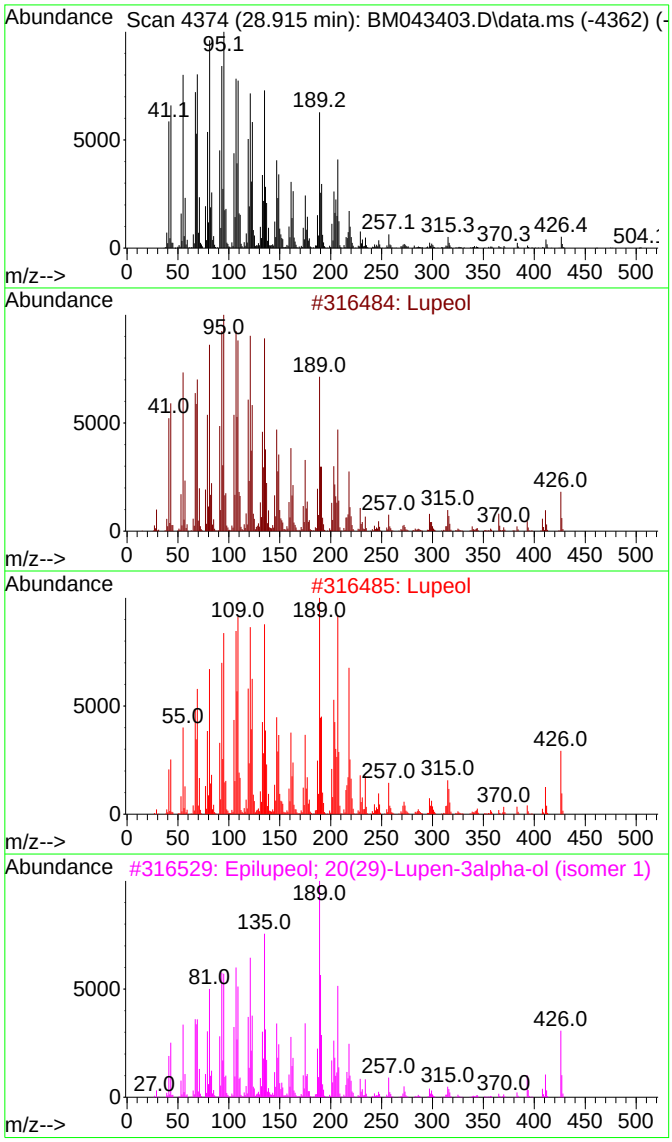
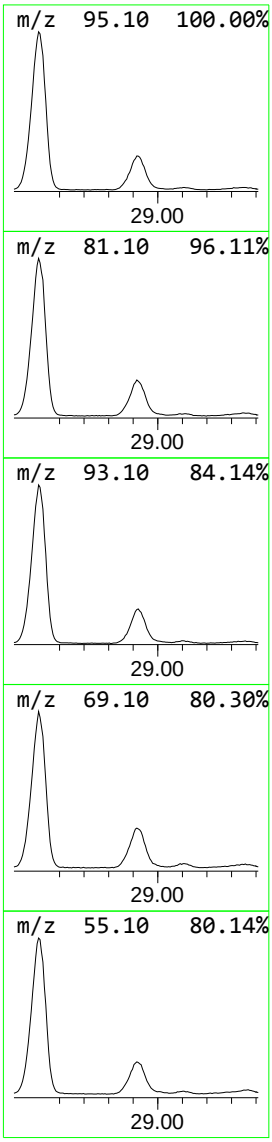
Peak Number 28 Lupeol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.915	46.11 ng/ul	10311500	Perylene-d12	23.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lupeol	426	C30H50O	000545-47-1	94
2	Lupeol	426	C30H50O	000545-47-1	93
3	Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-3	90
4	Lupeol, trifluoroacetate	522	C32H49F3O2	1000394-56-7	81
5	Uvidin C	254	C15H26O3	074635-85-1	70





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM121823\
Data File : BM043403.D
Acq On : 18 Dec 2023 21:10
Operator : MA/JU
Sample : 05807-03
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0AX5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzaldehyde, 3...	13.557	2.1	ng/ul	502229	3	14.621	4785220	20.0
n-Hexadecanoic ...	18.268	7.9	ng/ul	1901240	4	17.368	4826940	20.0
Tetradecane, 1-...	20.304	3.8	ng/ul	1021140	5	21.539	5362570	20.0
unknown-01	20.956	5.4	ng/ul	1456320	5	21.539	5362570	20.0
unknown-02	21.027	6.1	ng/ul	1626130	5	21.539	5362570	20.0
unknown-03	21.145	57.0	ng/ul	15283400	5	21.539	5362570	20.0
unknown-04	21.192	4.7	ng/ul	1267530	5	21.539	5362570	20.0
Pentadecafluoro...	21.262	27.6	ng/ul	7408260	5	21.539	5362570	20.0
unknown-05	21.286	36.3	ng/ul	9718480	5	21.539	5362570	20.0
Sesquirosefuran	21.445	10.5	ng/ul	2811040	5	21.539	5362570	20.0
n-Tetracosanol-1	22.198	29.8	ng/ul	8001270	5	21.539	5362570	20.0
Supraene	22.827	4.0	ng/ul	905106	6	23.968	4472850	20.0
(DEL) Alkane: S...	23.262	17.7	ng/ul	3949260	6	23.968	4472850	20.0
1-Heneicosanol	23.303	27.9	ng/ul	6250420	6	23.968	4472850	20.0
2-Heptacosanone	23.409	3.1	ng/ul	689235	6	23.968	4472850	20.0
.gamma.-Tocopherol	24.503	4.6	ng/ul	1025880	6	23.968	4472850	20.0
(DEL) Alkane: S...	24.650	7.8	ng/ul	1749430	6	23.968	4472850	20.0
1-Docosanol, me...	24.744	21.2	ng/ul	4747610	6	23.968	4472850	20.0
unknown-06	24.874	10.4	ng/ul	2320870	6	23.968	4472850	20.0
1,6-Naphthyridi...	25.415	7.4	ng/ul	1652790	6	23.968	4472850	20.0
unknown-07	26.003	12.2	ng/ul	2717480	6	23.968	4472850	20.0
Heptacosyl acetate	26.709	9.1	ng/ul	2031800	6	23.968	4472850	20.0
1H-Cycloprop[e]...	27.656	27.9	ng/ul	6239230	6	23.968	4472850	20.0
Lup-20(29)-en-3...	28.515	201.0	ng/ul	44947800	6	23.968	4472850	20.0
Lupeol	28.915	46.1	ng/ul	10311500	6	23.968	4472850	20.0