LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013261.D
Acq On : 23 Dec 2022 00:43
Operator : CG/JU
Sample : N6015-20
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBXZ9

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_P\Methods\SFAM-EPA-BP120722.M
Title : SVOA CALIBRATION

Signal : TIC: BP013261.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.334	21	25	31	rVB	139546	170025	0.46%	0.092%
2	3.764	95	98	113	rBV	1501947	2234627	6.10%	1.206%
3	4.087	150	153	163	rVB	54343	73589	0.20%	0.040%
4	5.040	309	315	320	rBV4	25648	48482	0.13%	0.026%
5	5.264	348	353	366	rVB	70218	123310	0.34%	0.067%
6	6.616	576	583	591	rVB	389304	577508	1.58%	0.312%
7	6.922	625	635	641	rBV7	35693	68436	0.19%	0.037%
8	7.105	660	666	676	rBV	2035666	3236026	8.83%	1.746%
9	7.269	688	694	707	rVB	1702734	2665513	7.27%	1.438%
10	7.475	722	729	738	rBV	2219798	3388538	9.24%	1.829%
11	7.946	801	809	816	rBV	2402723	3777844	10.31%	2.039%
12	8.658	922	930	940	rBV	2056360	3314427	9.04%	1.789%
13	9.110	999	1007	1018	rBV	1978629	3347795	9.13%	1.807%
14	9.269	1029	1034	1041	rVB6	21983	40262	0.11%	0.022%
15	9.516	1070	1076	1084	rBV	57456	98826	0.27%	0.053%
16	9.840	1122	1131	1143	rBV	1706113	2858303	7.80%	1.542%
17	10.069	1164	1170	1177	rVB9	26842	58642	0.16%	0.032%
18	10.381	1215	1223	1236	rBV	2644230	4482273	12.23%	2.419%
19	10.757	1279	1287	1295	rBV	3264685	5341938	14.57%	2.883%
20	10.899	1304	1311	1329	rBV	1880527	3238367	8.83%	1.748%
21	12.163	1522	1526	1533	rBV2	32823	49933	0.14%	0.027%
22	12.340	1552	1556	1562	rBV	41275	71430	0.19%	0.039%
23	13.398	1730	1736	1741	rVV	71426	120463	0.33%	0.065%
24	13.457	1741	1746	1752	rVV4	58680	98792	0.27%	0.053%
25	13.510	1752	1755	1760	rVV3	26421	49157	0.13%	0.027%
26	13.904	1817	1822	1829	rBV	240845	347491	0.95%	0.188%
27	13.993	1829	1837	1846	rBV	4332119	5998505	16.36%	3.237%
28	14.110	1853	1857	1862	rVB6	43015	61203	0.17%	0.033%
29	14.281	1879	1886	1895	rBV	5079058	7363319	20.09%	3.973%
30	14.422	1904	1910	1915	rBV3	53713	84287	0.23%	0.045%
31	14.469	1915	1918	1923	rVB2	40355	55913	0.15%	0.030%
32	14.540	1925	1930	1932	rBV4	57254	81623	0.22%	0.044%
33	14.587	1932	1938	1945	rVV	4473384	6538930	17.84%	3.529%
34	14.651	1945	1949	1953	rVV2	153669	259029	0.71%	0.140%
35	14.692	1953	1956	1961	rVB5	63237	99758	0.27%	0.054%
36	14.787	1966	1972	1977	rBV	1258559	1973351	5.38%	1.065%

LSC Area Percent Report

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Operator : CG/JU
Sample : N6015-20
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ9

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_P\Methods\SFAM-EPA-BP120722.M
Title : SVOA CALIBRATION

37	14.828	1977	1979	1990	rVB2	336420	529629	1.44%	0.286%
38	14.940	1995	1998	2003	rVV5	49802	77984	0.21%	0.042%
39	14.992	2003	2007	2012	rVV4	60343	102894	0.28%	0.056%
40	15.040	2012	2015	2020	rVV5	35245	57305	0.16%	0.031%
41	15.498	2084	2093	2100	rBV	266691	395350	1.08%	0.213%
42	15.581	2100	2107	2119	rBV	6201208	8854523	24.16%	4.778%
43	15.698	2121	2127	2136	rBV	1213069	1689693	4.61%	0.912%
44	15.822	2144	2148	2155	rVB5	55136	86081	0.23%	0.046%
45	15.945	2164	2169	2177	rVB	1290017	1740059	4.75%	0.939%
46	16.028	2178	2183	2184	rBV	169074	197254	0.54%	0.106%
47	16.051	2184	2187	2197	rVB4	212501	364516	0.99%	0.197%
48	16.157	2199	2205	2211	rBV	402971	561546	1.53%	0.303%
49	16.516	2262	2266	2272	rVB3	52248	77105	0.21%	0.042%
50	16.728	2298	2302	2307	rBV	120271	170904	0.47%	0.092%
51	17.092	2360	2364	2367	rBV6	23783	36660	0.10%	0.020%
52	17.134	2369	2371	2381	rVB10	24383	56790	0.15%	0.031%
53	17.228	2383	2387	2392	rBV2	68730	103542	0.28%	0.056%
54	17.292	2394	2398	2401	rBV3	47822	72462	0.20%	0.039%
55	17.345	2401	2407	2417	rVV	4458955	6649764	18.14%	3.588%
56	17.445	2417	2424	2431	rVV	5507342	7680121	20.95%	4.144%
57	17.504	2431	2434	2438	rVB2	52866	69113	0.19%	0.037%
58	17.698	2463	2467	2469	rBV5	57524	72940	0.20%	0.039%
59	18.092	2530	2534	2540	rBV2	120820	227073	0.62%	0.123%
60	18.157	2542	2545	2550	rVV2	131314	181687	0.50%	0.098%
61	18.216	2550	2555	2569	rBV	1697216	2491553	6.80%	1.345%
62	18.504	2601	2604	2608	rBV6	37498	66590	0.18%	0.036%
63	18.551	2608	2612	2619	rVV3	96171	175696	0.48%	0.095%
64	19.251	2729	2731	2737	rVB	80794	103440	0.28%	0.056%
65	19.333	2738	2745	2746	rBV4	221093	438174	1.20%	0.236%
66	19.445	2761	2764	2777	rVB	239820	354137	0.97%	0.191%
67	19.680	2798	2804	2813	rBV	6465636	8816702	24.05%	4.758%
68	21.127	3046	3050	3060	rBV	1532253	1972425	5.38%	1.064%
69	21.433	3097	3102	3107	rBV	5061971	6593543	17.99%	3.558%
70	22.704	3314	3318	3327	rVB	1288077	1951441	5.32%	1.053%
71	23.127	3386	3390	3396	rBV2	957573	1486380	4.06%	0.802%
72	23.757	3490	3497	3512	rVB2	4940411	10809189	29.49%	5.833%
73	23.916	3518	3524	3538	rVB2	3550789	7443786	20.31%	4.017%
74	24.533	3624	3629	3636	rVB	1381962	2861722	7.81%	1.544%
75	24.633	3641	3646	3659	rVB	1022220	2681858	7.32%	1.447%
76	27.462	4120	4127	4148	rVB3	2073082	7958217	21.71%	4.294%

LSC Area Percent Report

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Sample : N6015-20
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DBXZ9

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

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Title : SVOA CALIBRATION

77	28.509	4293	4305	4324	rVB2	8724525	36654614	100.00%	19.780%

Sum of corrected areas: 185312377

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
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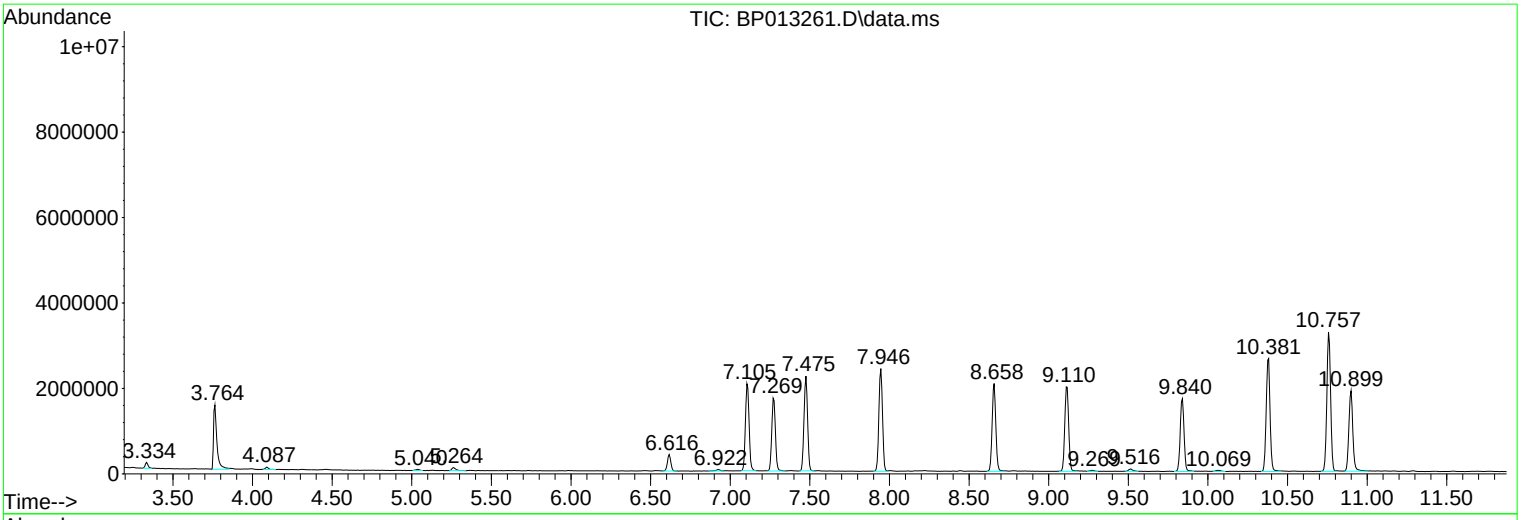
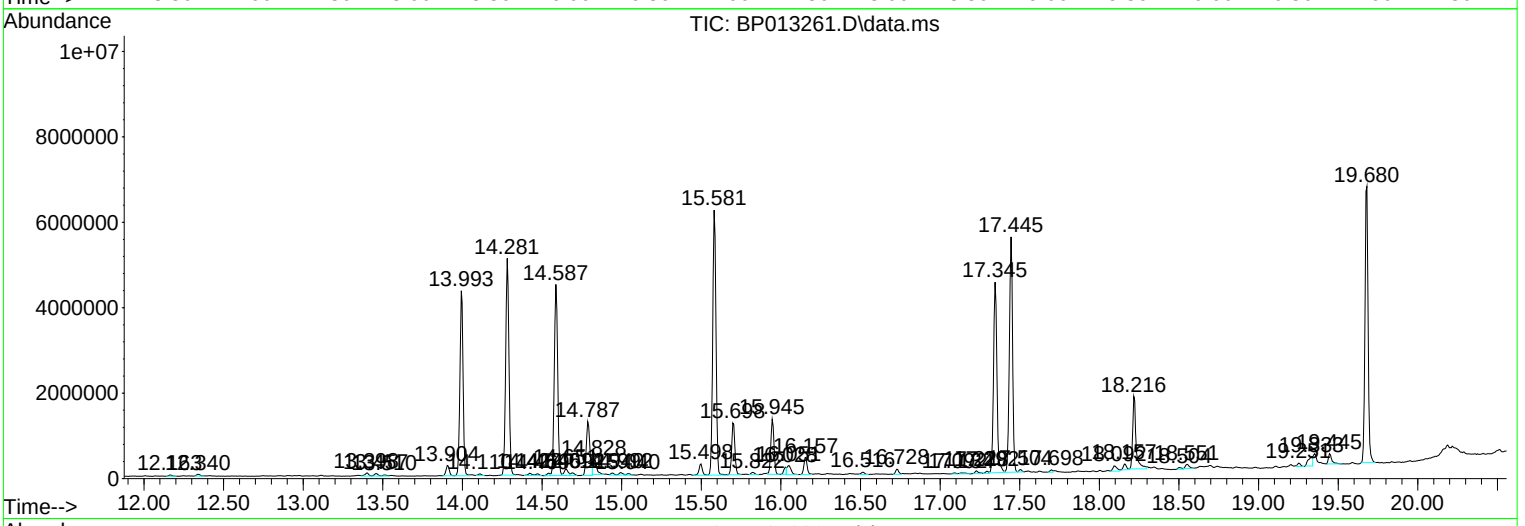
Acq On : 23 Dec 2022 00:43
Operator : CG/JU
Sample : N6015-20
Misc :
ALS Vial : 28 Sample Multiplier: 1

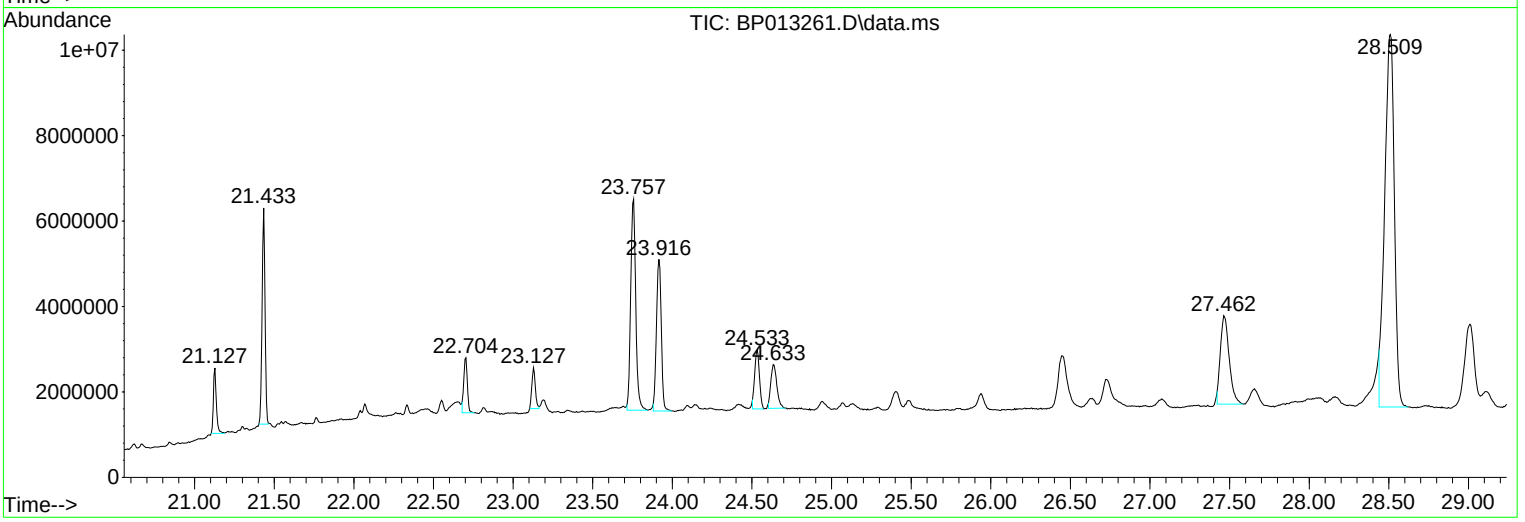
Instrument :
BNA_P
ClientSampleId :
DBXZ9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013261.D
Acq On : 23 Dec 2022 00:43
Operator : CG/JU
Sample : N6015-20
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

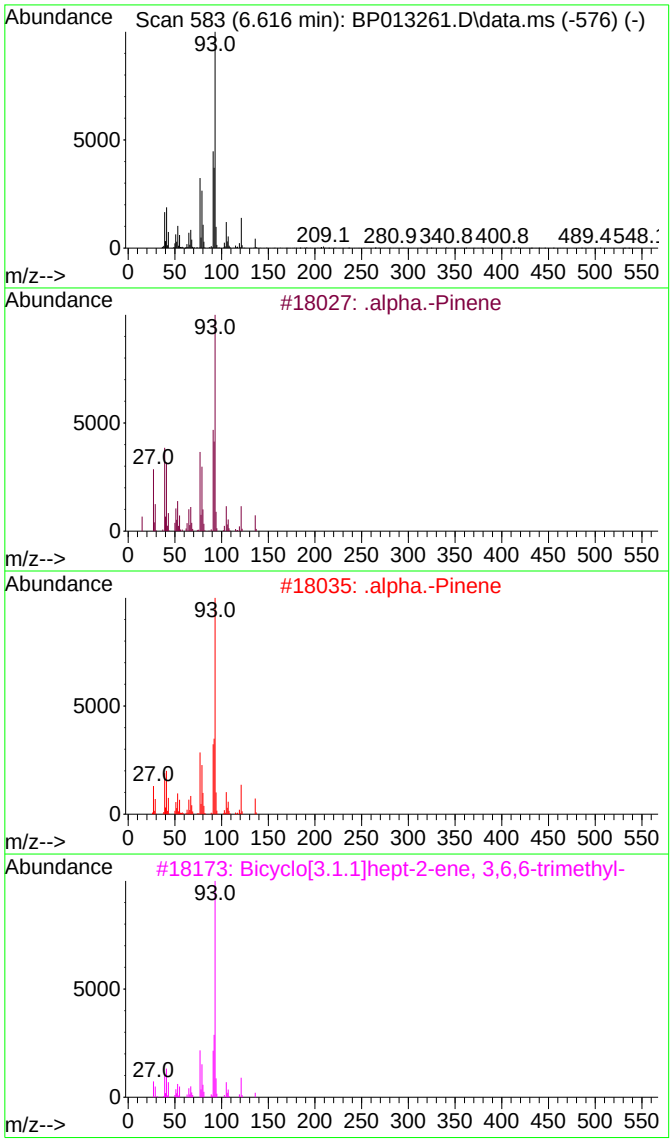
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

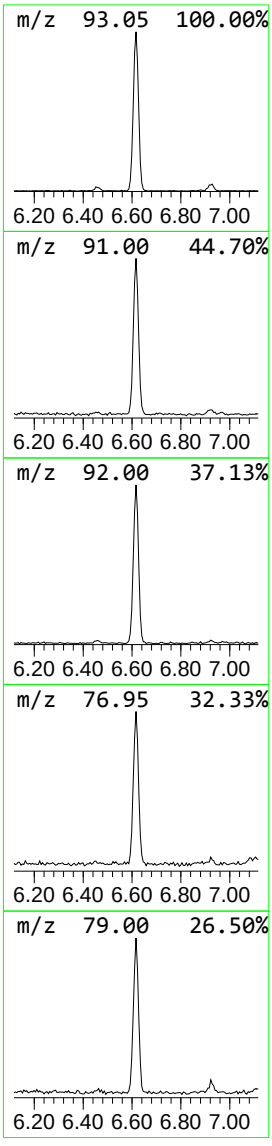
****

Peak Number 1 .alpha.-Pinene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.616	3.06 ng/ul	577508	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	94
2	.alpha.-Pinene	136	C10H16	000080-56-8	94
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	94
4	trans-.beta.-Ocimene	136	C10H16	003779-61-1	91
5	3-Carene	136	C10H16	013466-78-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013261.D
Acq On : 23 Dec 2022 00:43
Operator : CG/JU
Sample : N6015-20
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

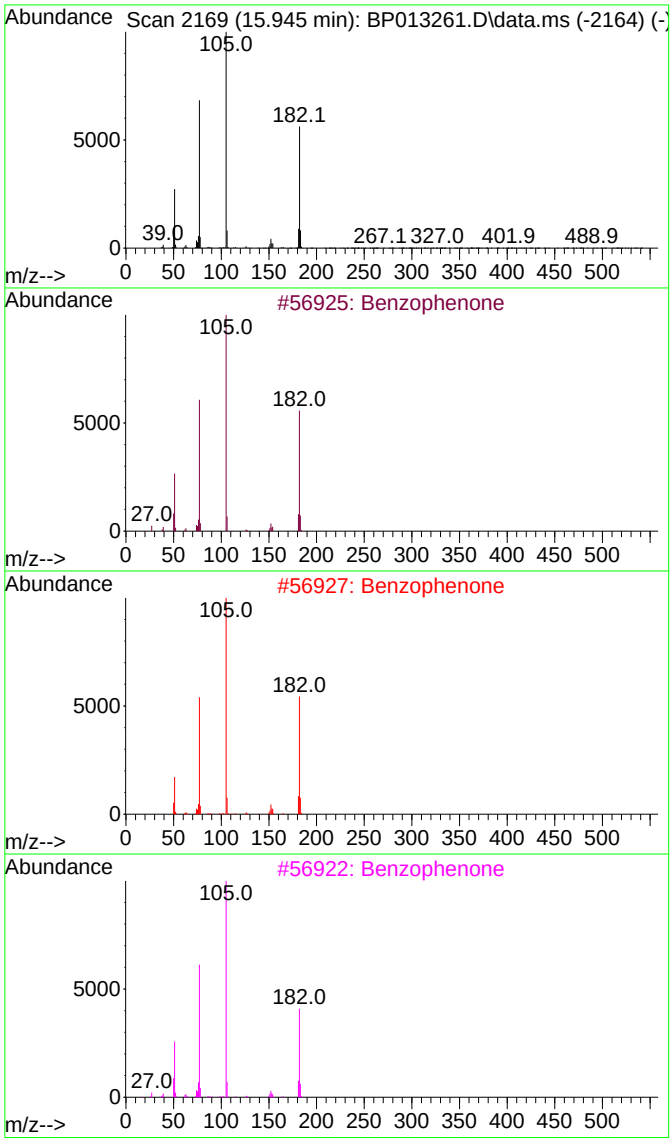
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

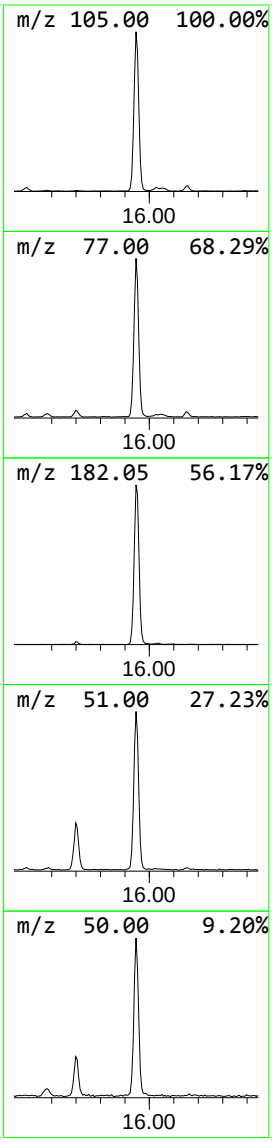
****

Peak Number 2 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	5.32 ng/ul	1740060	Acenaphthene-d10	14.587

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	95
3	Benzophenone	182	C13H10O	000119-61-9	94
4	Benzophenone	182	C13H10O	000119-61-9	90
5	Benzophenone	182	C13H10O	000119-61-9	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013261.D
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Sample : N6015-20
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

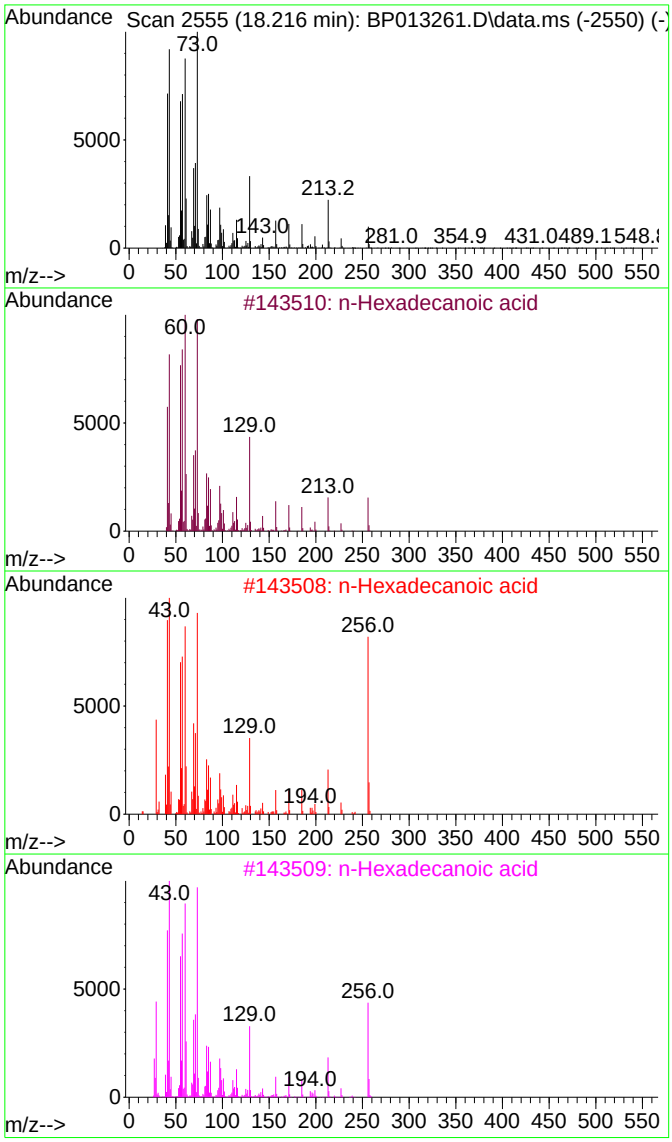
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

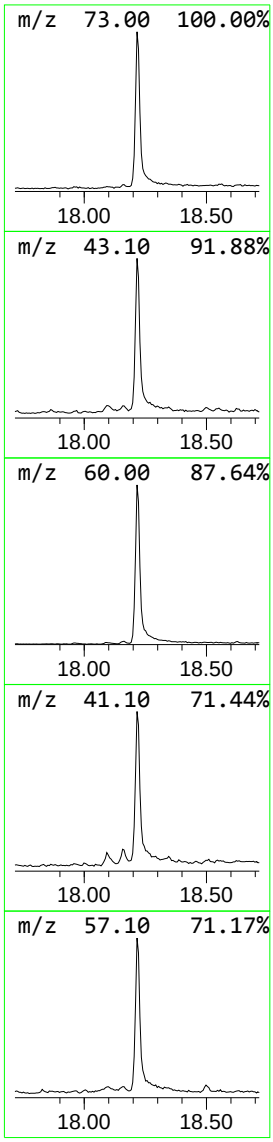
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	7.49 ng/ul	2491550	Phenanthrene-d10	17.345

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	97
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
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ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
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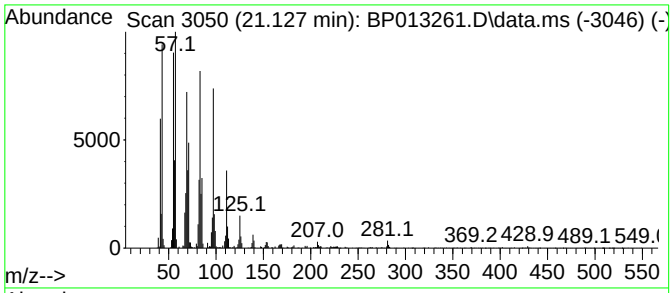
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

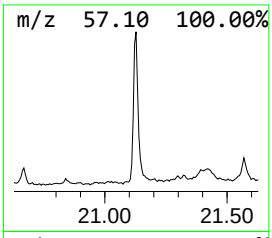
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

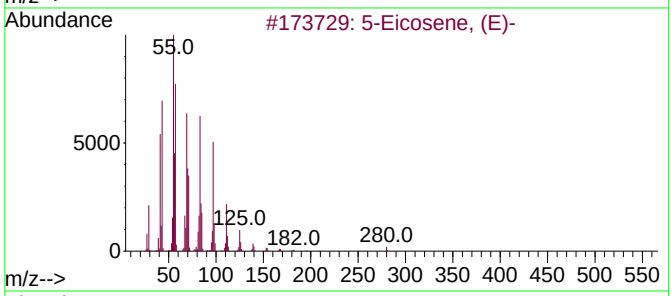
****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

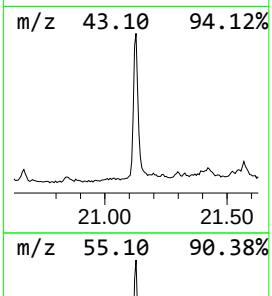
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	5.98 ng/ul	1972430	Chrysene-d12	21.433

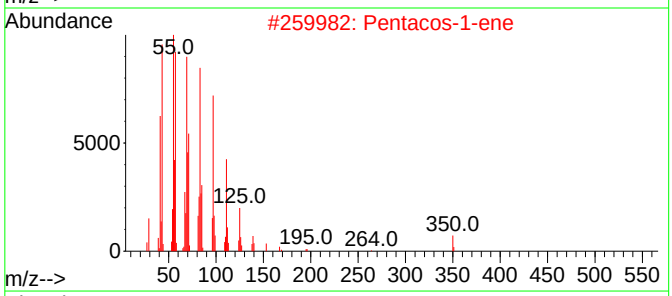
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	Pentacos-1-ene	350	C25H50	016980-85-1	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	1-Hexacosene	364	C26H52	018835-33-1	94

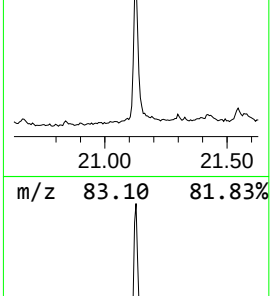


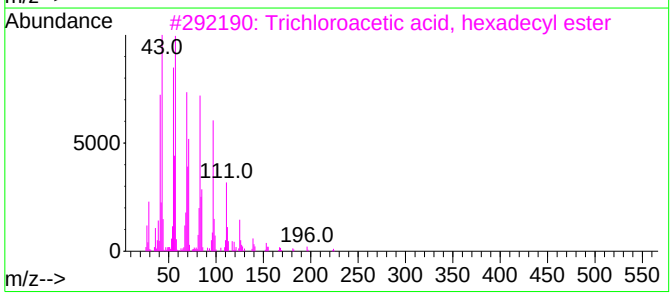












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013261.D
Acq On : 23 Dec 2022 00:43
Operator : CG/JU
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Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

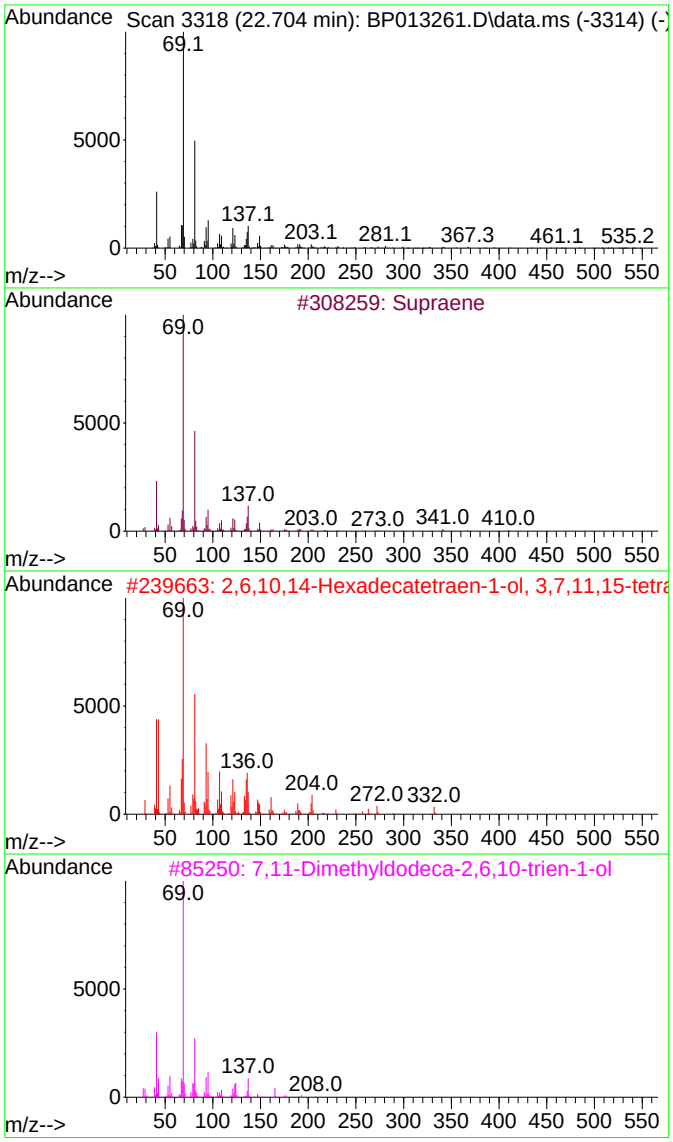
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

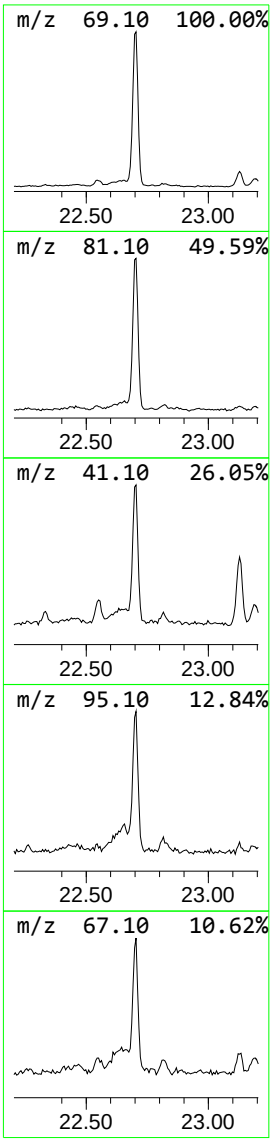
****

Peak Number 5 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.704	5.24 ng/ul	1951440	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	78
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	trans-Farnesol	222	C15H26O	000106-28-5	64
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50





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Acq On : 23 Dec 2022 00:43
Operator : CG/JU
Sample : N6015-20
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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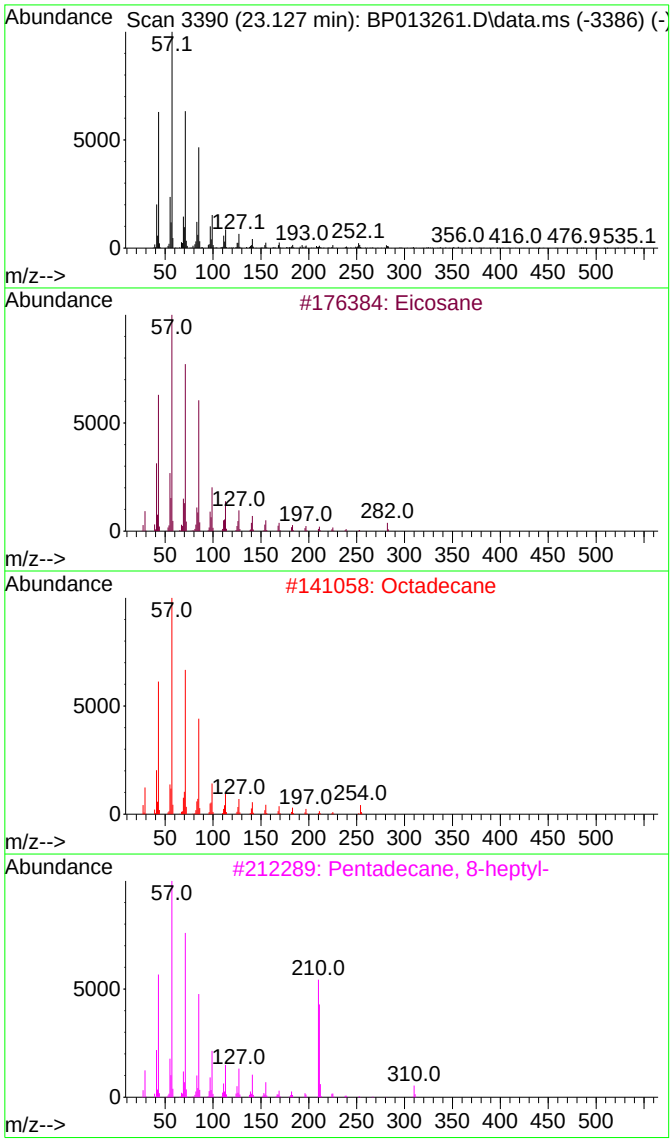
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

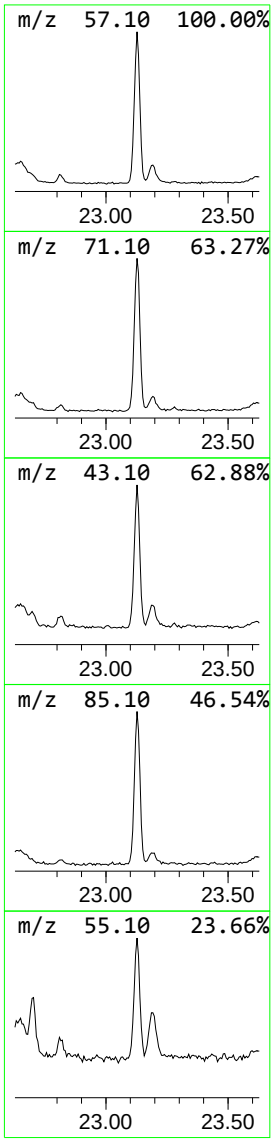
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.127	3.99 ng/ul	1486380	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Octadecane	254	C18H38	000593-45-3	94
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	94
4	Docosane	310	C22H46	000629-97-0	93
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93





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Acq On : 23 Dec 2022 00:43
Operator : CG/JU
Sample : N6015-20
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ9

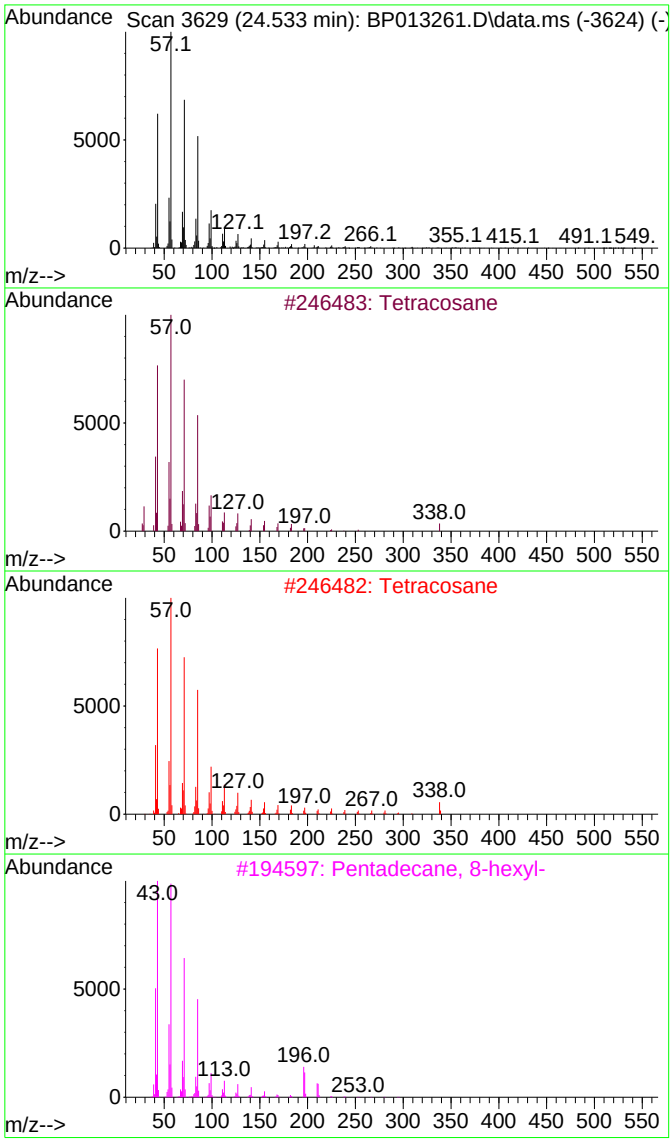
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

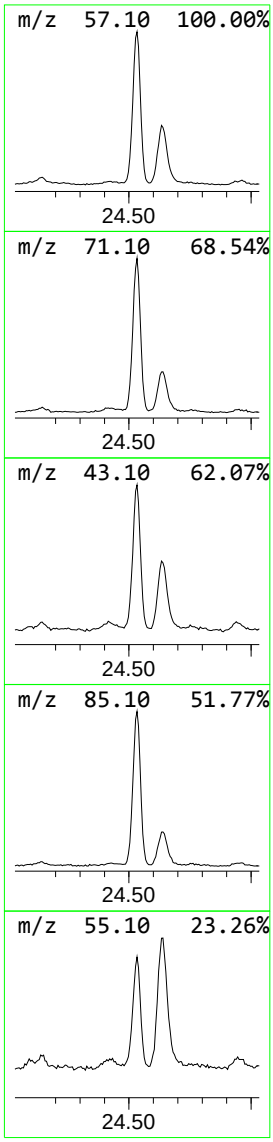
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.533	7.69 ng/ul	2861720	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	98
2	Tetracosane	338	C24H50	000646-31-1	96
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
4	Octadecane	254	C18H38	000593-45-3	93
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93





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Operator : CG/JU
Sample : N6015-20
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

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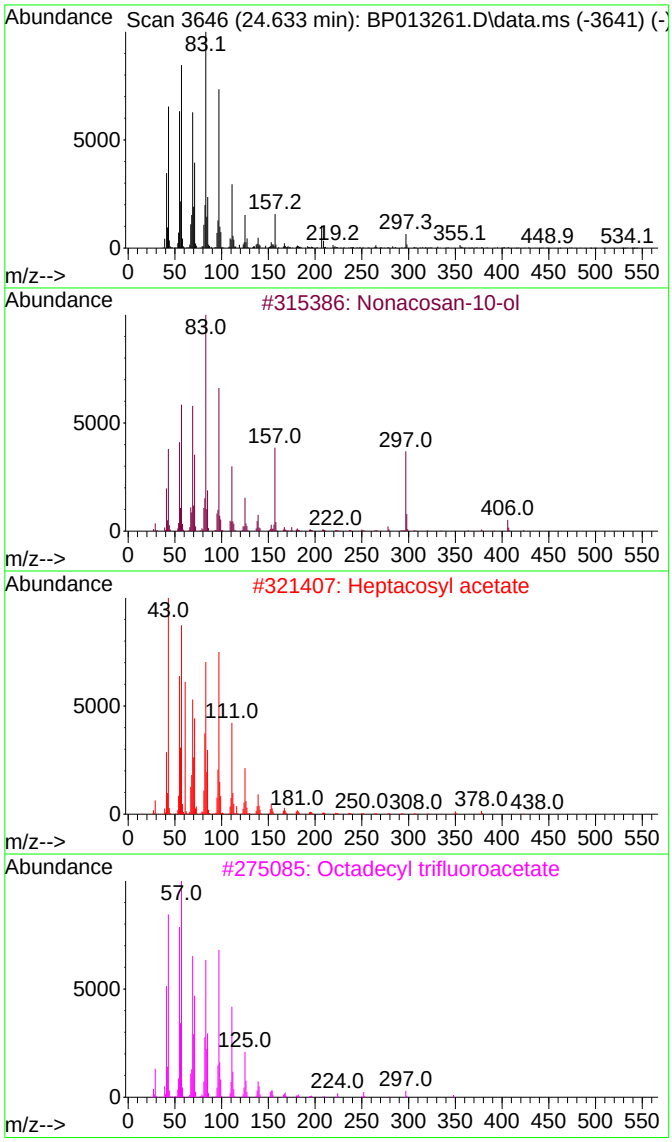
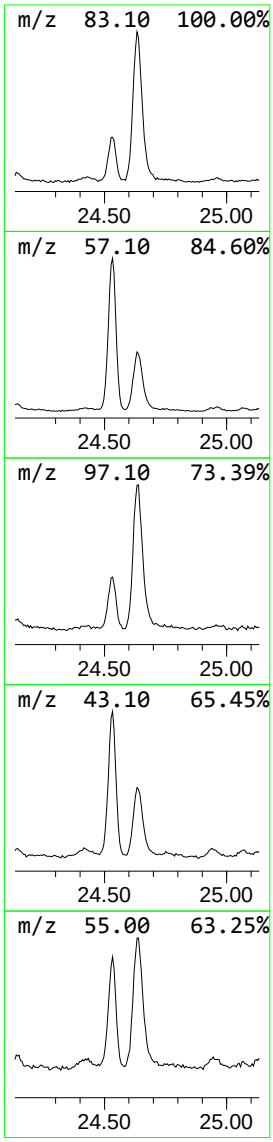
Peak Number 8 Nonacosan-10-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.633	7.21 ng/ul	2681860	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacosan-10-ol	424	C29H60O	000504-55-2	86
2	Heptacosyl acetate	438	C29H58O2	1000351-78-2	60
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	46
4	Propyl triacontyl ether	481	C33H68O	1000406-28-6	46
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	45





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Operator : CG/JU
Sample : N6015-20
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

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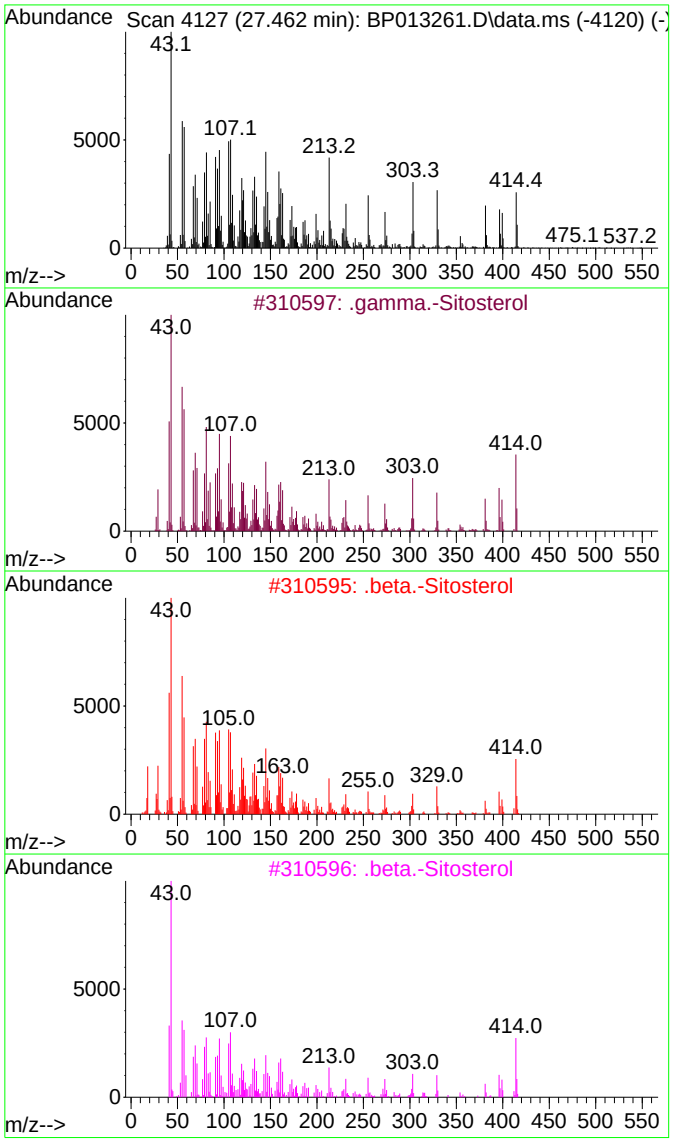
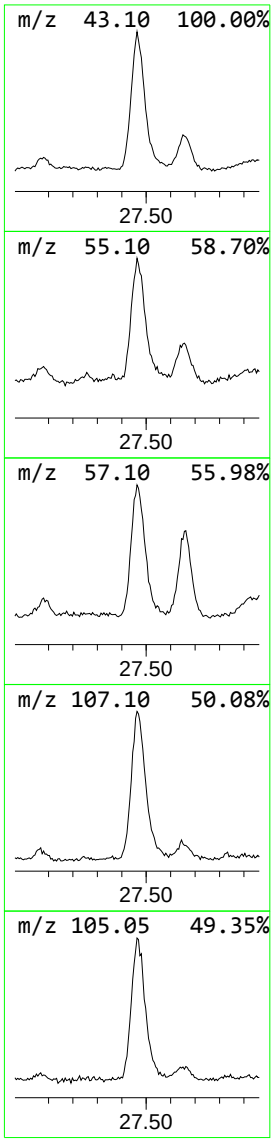
Peak Number 9 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.462	21.38 ng/ul	7958220	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	93
3	.beta.-Sitosterol	414	C29H50O	000083-46-5	89
4	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	55
5	.gamma.-Sitosterol	414	C29H50O	000083-47-6	55





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Data File : BP013261.D
Acq On : 23 Dec 2022 00:43
Operator : CG/JU
Sample : N6015-20
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXZ9

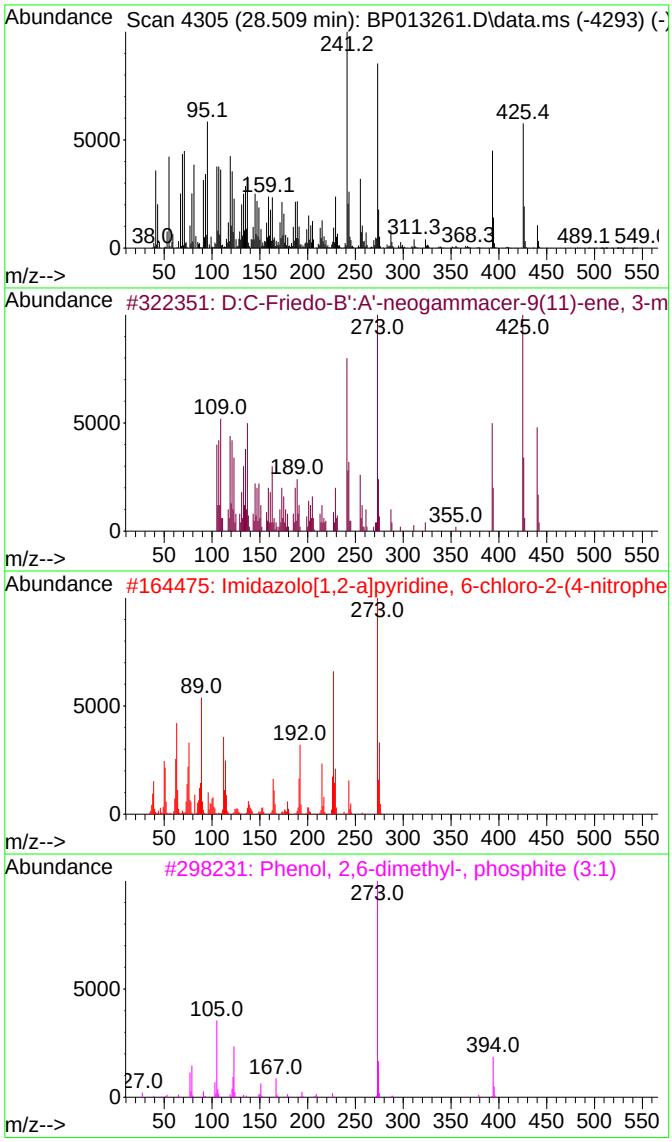
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

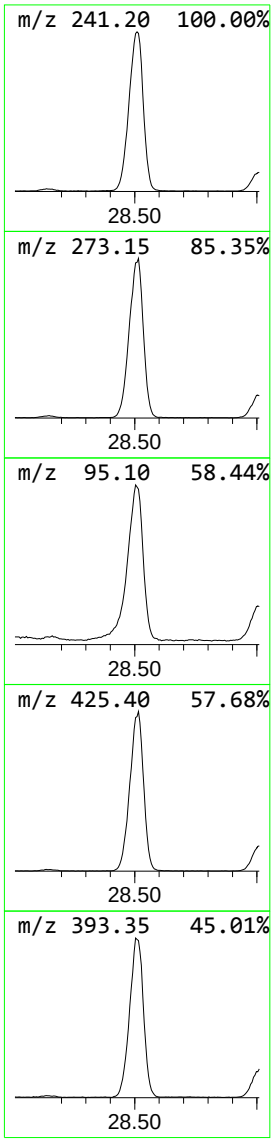
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 D:C-Friedo-B':A'-neogammace... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.509	98.48 ng/ul	36654600	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	58
2	Imidazolo[1,2-a]pyridine, 6-chlo...	273	C13H8ClN3O2	118000-62-7	53
3	Phenol, 2,6-dimethyl-, phosphite...	394	C24H27O3P	052830-49-6	25
4	Benzene, 1-[2-(2-chloroethoxy)et...	312	C18H29ClO2	065925-28-2	25
5	2-(Phenylmethyl)phenol, tert-but...	298	C19H26OSi	1417315-87-7	15





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013261.D
Acq On : 23 Dec 2022 00:43
Operator : CG/JU
Sample : N6015-20
Misc :
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Instrument :
BNA_P
ClientSampleId :
DBXZ9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.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
.alpha.-Pinene	6.616	3.1	ng/ul	577508	1	7.946	3777840	20.0
Benzophenone	15.945	5.3	ng/ul	1740060	3	14.587	6538930	20.0
n-Hexadecanoic ...	18.216	7.5	ng/ul	2491550	4	17.345	6649760	20.0
(DEL) Alkane: S...	21.127	6.0	ng/ul	1972430	5	21.433	6593540	20.0
Supraene	22.704	5.2	ng/ul	1951440	6	23.916	7443790	20.0
(DEL) Alkane: S...	23.127	4.0	ng/ul	1486380	6	23.916	7443790	20.0
(DEL) Alkane: S...	24.533	7.7	ng/ul	2861720	6	23.916	7443790	20.0
Nonacosan-10-ol	24.633	7.2	ng/ul	2681860	6	23.916	7443790	20.0
.gamma.-Sitosterol	27.462	21.4	ng/ul	7958220	6	23.916	7443790	20.0
D:C-Friedo-B':A...	28.509	98.5	ng/ul	36654600	6	23.916	7443790	20.0