LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013187.D
Acq On : 21 Dec 2022 03:18
Operator : CG/JU
Sample : N6009-04
Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB6

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: BP013187.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	22	25	36	rVB	87359	133404	1.24%	0.124%
2	3.628	72	75	82	rVB	41901	67177	0.63%	0.062%
3	3.781	98	101	113	rVV2	101845	154124	1.44%	0.143%
4	3.869	113	116	121	rVB	76210	100522	0.94%	0.093%
5	3.952	126	130	133	rBV5	16326	29989	0.28%	0.028%
6	3.999	134	138	145	rVB	63073	92821	0.87%	0.086%
7	4.093	151	154	160	rVB2	32106	48568	0.45%	0.045%
8	4.469	216	218	226	rVB7	15598	28002	0.26%	0.026%
9	4.664	248	251	254	rVB4	13473	15252	0.14%	0.014%
10	5.034	309	314	323	rVB3	51983	114741	1.07%	0.106%
11	5.134	327	331	336	rVB6	15138	24544	0.23%	0.023%
12	6.622	577	584	592	rVV	497717	767964	7.16%	0.712%
13	6.928	633	636	641	rBV6	16440	23594	0.22%	0.022%
14	7.110	659	667	679	rVB	1216595	1914797	17.86%	1.775%
15	7.275	689	695	703	rVB	1158113	1813968	16.92%	1.682%
16	7.387	708	714	722	rVB	188310	312924	2.92%	0.290%
17	7.481	723	730	739	rBV	1391793	2139744	19.96%	1.984%
18	7.563	739	744	754	rVV7	21038	39626	0.37%	0.037%
19	7.952	802	810	818	rBV	1667456	2585173	24.12%	2.396%
20	8.010	818	820	827	rVV5	12243	18669	0.17%	0.017%
21	8.169	841	847	852	rBV7	16917	32975	0.31%	0.031%
22	8.228	852	857	861	rVB	59862	90019	0.84%	0.083%
23	8.663	924	931	940	rBV	566922	919767	8.58%	0.853%
24	8.781	946	951	958	rVB	76295	123806	1.16%	0.115%
25	9.122	1001	1009	1016	rBV	1294062	2143708	20.00%	1.987%
26	9.522	1069	1077	1088	rVB	47218	83772	0.78%	0.078%
27	9.846	1124	1132	1145	rBV	1110717	1823161	17.01%	1.690%
28	9.999	1151	1158	1164	rBV10	10078	24551	0.23%	0.023%
29	10.175	1183	1188	1191	rBV6	10761	16305	0.15%	0.015%
30	10.387	1216	1224	1234	rBV	1539447	2586134	24.13%	2.397%
31	10.546	1245	1251	1261	rBV2	65865	118850	1.11%	0.110%
32	10.763	1281	1288	1295	rBV	2096122	3609168	33.67%	3.346%
33	10.822	1295	1298	1305	rVB4	37309	54812	0.51%	0.051%
34	10.904	1305	1312	1324	rBV	880790	1564373	14.59%	1.450%
35	11.240	1364	1369	1373	rVB8	8310	13476	0.13%	0.012%
36	11.298	1373	1379	1386	rBV8	13408	27108	0.25%	0.025%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
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Acq On : 21 Dec 2022 03:18
Operator : CG/JU
Sample : N6009-04
Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB6

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	11.551	1417	1422	1427	rBV9	10242	19768	0.18%	0.018%
38	12.016	1497	1501	1506	rVB8	8569	14366	0.13%	0.013%
39	12.175	1524	1528	1533	rVB3	16887	25902	0.24%	0.024%
40	12.257	1537	1542	1544	rBV4	8779	13849	0.13%	0.013%
41	12.351	1552	1558	1562	rVB	27707	46690	0.44%	0.043%
42	12.751	1621	1626	1631	rBV9	8071	16611	0.15%	0.015%
43	13.122	1685	1689	1696	rVV10	8463	14612	0.14%	0.014%
44	13.192	1696	1701	1705	rVB8	9081	13375	0.12%	0.012%
45	13.410	1731	1738	1743	rVB	51535	84286	0.79%	0.078%
46	13.487	1743	1751	1755	rBV6	23671	60834	0.57%	0.056%
47	13.916	1817	1824	1831	rBV	147473	220375	2.06%	0.204%
48	13.998	1831	1838	1848	rBV	2899959	3938101	36.74%	3.651%
49	14.110	1853	1857	1861	rVV6	15524	25469	0.24%	0.024%
50	14.181	1866	1869	1874	rVB7	7966	12132	0.11%	0.011%
51	14.234	1874	1878	1880	rBV5	8463	14875	0.14%	0.014%
52	14.287	1880	1887	1900	rBV	3282571	4772879	44.53%	4.424%
53	14.481	1916	1920	1924	rVB2	29528	41999	0.39%	0.039%
54	14.545	1927	1931	1933	rBV5	13833	21312	0.20%	0.020%
55	14.592	1933	1939	1946	rVV	3097970	4546231	42.41%	4.214%
56	14.657	1946	1950	1954	rVV3	34506	59956	0.56%	0.056%
57	14.692	1954	1956	1965	rVB8	22046	42015	0.39%	0.039%
58	14.792	1966	1973	1978	rBV	741710	1170575	10.92%	1.085%
59	14.834	1978	1980	1992	rVV2	107590	204406	1.91%	0.189%
60	14.945	1995	1999	2004	rVV3	42182	66639	0.62%	0.062%
61	15.010	2004	2010	2015	rVB6	36189	69619	0.65%	0.065%
62	15.386	2070	2074	2076	rBV5	8217	12514	0.12%	0.012%
63	15.475	2085	2089	2092	rBV3	30666	49501	0.46%	0.046%
64	15.504	2092	2094	2100	rVB5	40218	48422	0.45%	0.045%
65	15.586	2100	2108	2115	rBV	4367259	6030966	56.26%	5.591%
66	15.704	2122	2128	2140	rBV	982731	1358970	12.68%	1.260%
67	15.828	2145	2149	2156	rVB5	26708	42769	0.40%	0.040%
68	15.910	2159	2163	2165	rBV	13044	17490	0.16%	0.016%
69	15.951	2165	2170	2178	rVB	417536	551529	5.15%	0.511%
70	16.034	2180	2184	2186	rBV2	37310	49056	0.46%	0.045%
71	16.157	2200	2205	2212	rVB2	83162	119349	1.11%	0.111%
72	16.292	2226	2228	2233	rBV6	10838	14571	0.14%	0.014%
73	16.439	2247	2253	2255	rBV6	12911	20451	0.19%	0.019%
74	16.733	2300	2303	2307	rVB6	12541	16470	0.15%	0.015%
75	16.881	2324	2328	2337	rVB2	59697	94658	0.88%	0.088%
76	17.228	2383	2387	2391	rBV7	32338	45276	0.42%	0.042%

LSC Area Percent Report

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Data File : BP013187.D
Acq On : 21 Dec 2022 03:18
Operator : CG/JU
Sample : N6009-04
Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB6

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	17.292	2396	2398	2401	rBV4	12033	15209	0.14%	0.014%
78	17.351	2401	2408	2413	rBV	3635534	5196627	48.48%	4.817%
79	17.451	2418	2425	2437	rVV	4064042	5911821	55.15%	5.480%
80	17.539	2438	2440	2450	rVB7	33318	61991	0.58%	0.057%
81	17.728	2469	2472	2478	rVB7	22856	37324	0.35%	0.035%
82	18.004	2516	2519	2523	rVB6	25350	30858	0.29%	0.029%
83	18.104	2532	2536	2542	rBV9	21854	34743	0.32%	0.032%
84	18.163	2542	2546	2550	rBV4	31127	36283	0.34%	0.034%
85	18.222	2551	2556	2562	rBV	566820	790595	7.38%	0.733%
86	18.557	2610	2613	2615	rBV4	26091	32974	0.31%	0.031%
87	18.627	2622	2625	2630	rVB	203938	229773	2.14%	0.213%
88	18.704	2634	2638	2642	rBV6	29784	44185	0.41%	0.041%
89	19.257	2729	2732	2738	rVB3	78155	104128	0.97%	0.097%
90	19.357	2738	2749	2755	rBV2	260246	583237	5.44%	0.541%
91	19.451	2761	2765	2772	rBV3	176754	256676	2.39%	0.238%
92	19.680	2798	2804	2817	rBV	6144442	8197818	76.48%	7.599%
93	21.127	3046	3050	3060	rBV	1168127	1527195	14.25%	1.416%
94	21.327	3082	3084	3088	rVB	210007	192979	1.80%	0.179%
95	21.433	3097	3102	3108	rBV	4596307	6429376	59.98%	5.960%
96	23.127	3386	3390	3397	rBV2	799226	1454612	13.57%	1.348%
97	23.757	3490	3497	3512	rVB	4373034	9431451	87.99%	8.743%
98	23.915	3518	3524	3542	rVB2	3436251	7156983	66.77%	6.634%
99	24.533	3624	3629	3638	rVB	851626	1753121	16.36%	1.625%
100	28.498	4295	4303	4325	rVB3	2815879	10718955	100.00%	9.936%

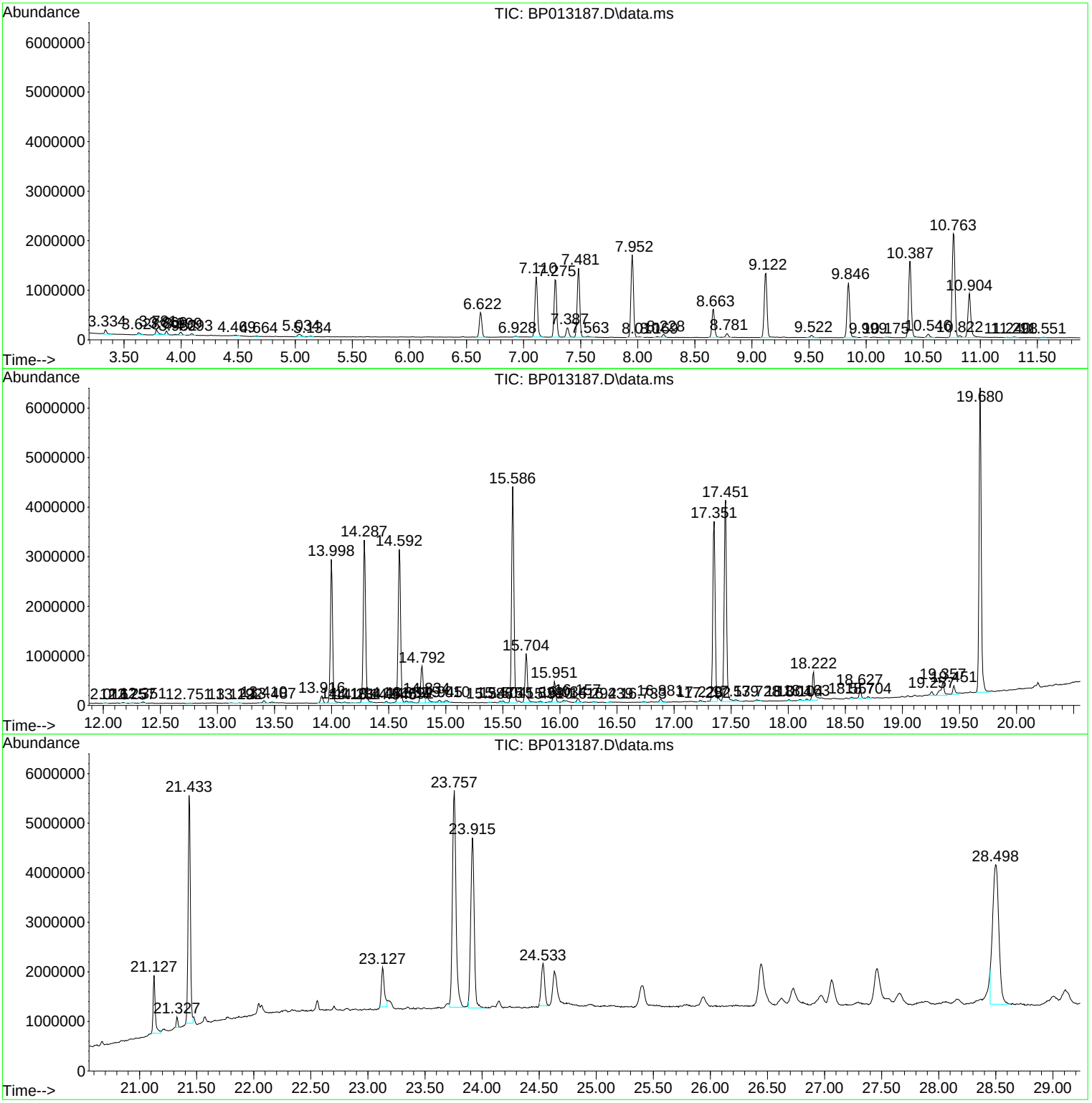
Sum of corrected areas: 107875370

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013187.D
Acq On : 21 Dec 2022 03:18
Operator : CG/JU
Sample : N6009-04
Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB6

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\BP121922\
Data File : BP013187.D
Acq On : 21 Dec 2022 03:18
Operator : CG/JU
Sample : N6009-04
Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB6

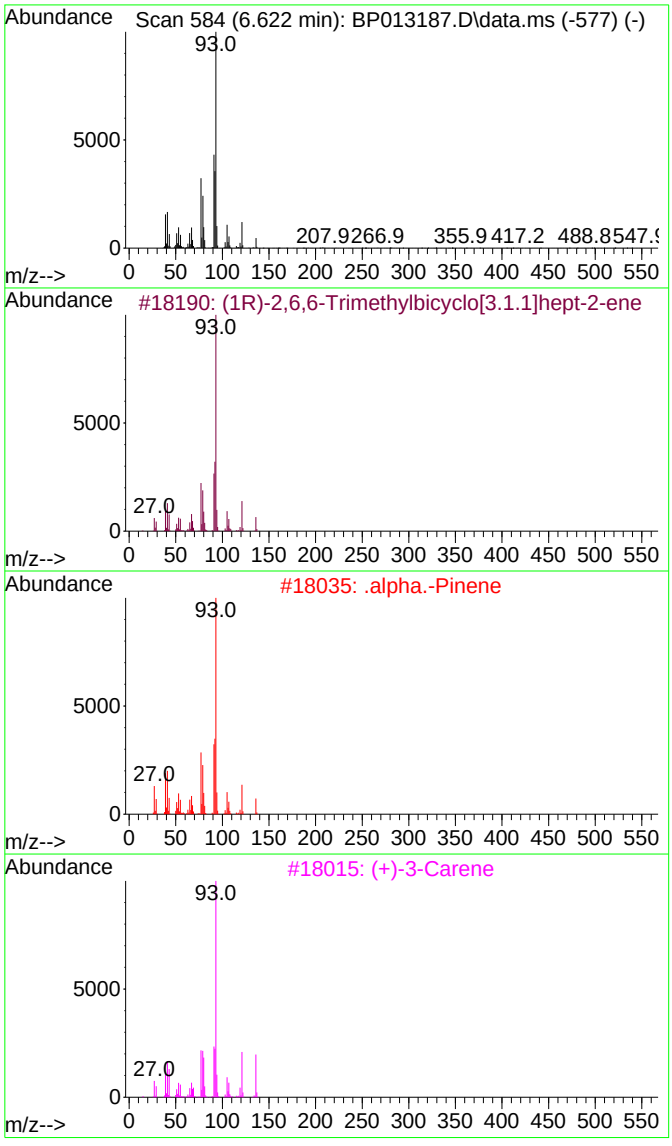
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

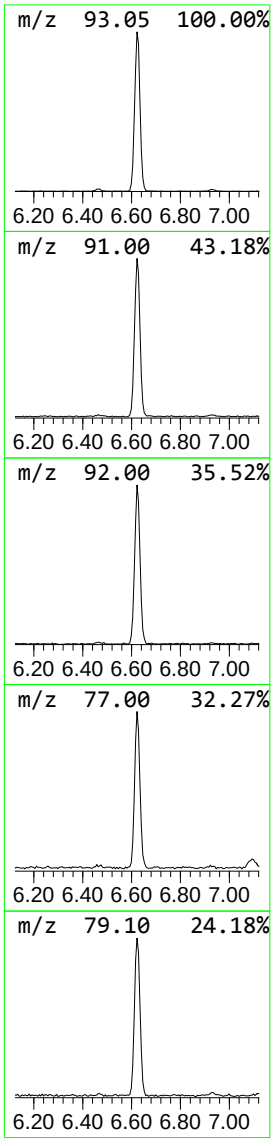
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.622	5.94 ng/ul	767964	1,4-Dichlorobenzene-d4	7.952

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	95
2	.alpha.-Pinene	136	C10H16	000080-56-8	94
3	(+)-3-Carene	136	C10H16	000498-15-7	91
4	3-Carene	136	C10H16	013466-78-9	91
5	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013187.D
Acq On : 21 Dec 2022 03:18
Operator : CG/JU
Sample : N6009-04
Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB6

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

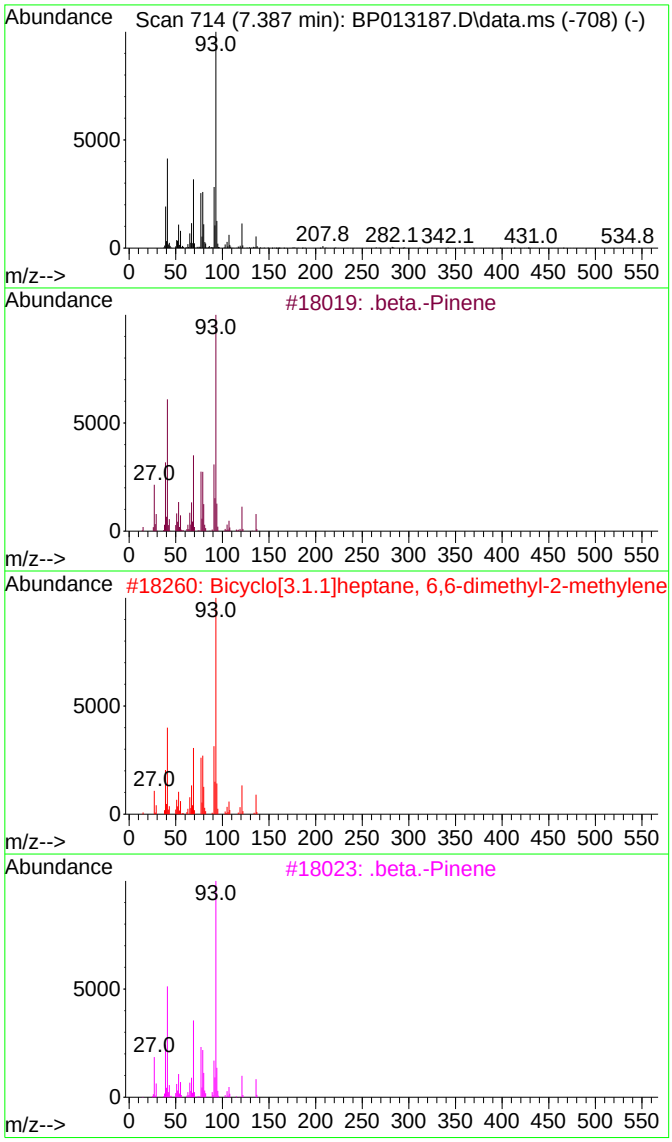
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

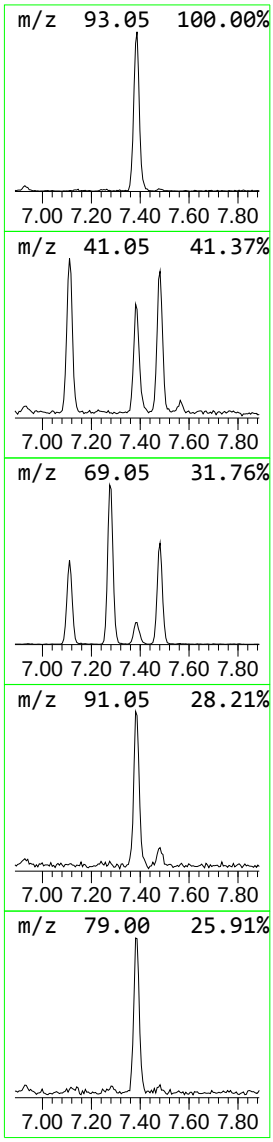
****

Peak Number 2 .beta.-Pinene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.387	2.42 ng/ul	312924	1,4-Dichlorobenzene-d4	7.952

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Pinene	136	C10H16	000127-91-3	96
2	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	91
3	.beta.-Pinene	136	C10H16	000127-91-3	91
4	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	91
5	.beta.-Pinene	136	C10H16	000127-91-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013187.D
Acq On : 21 Dec 2022 03:18
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Sample : N6009-04
Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB6

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

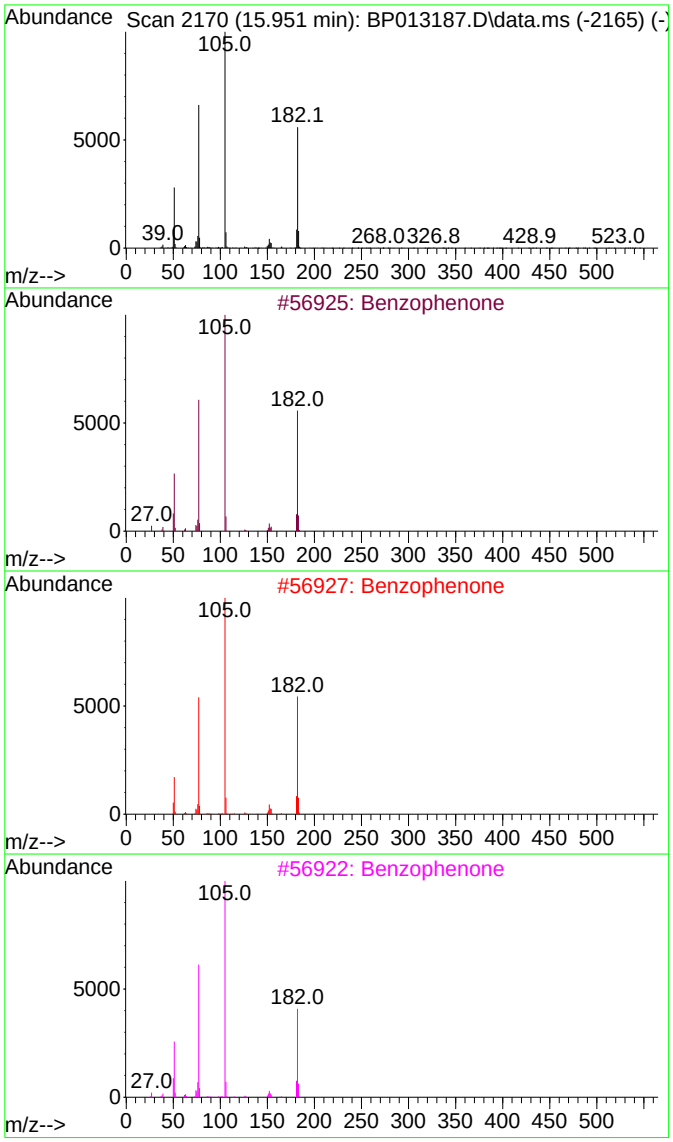
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

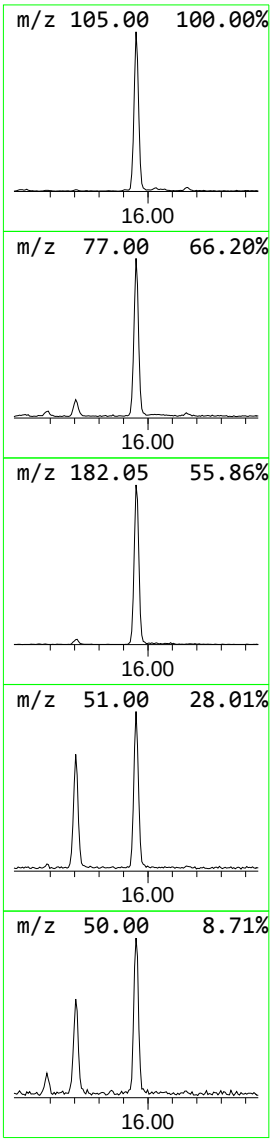
****

Peak Number 3 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	2.43 ng/ul	551529	Acenaphthene-d10	14.592

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	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013187.D
Acq On : 21 Dec 2022 03:18
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Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
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DBYB6

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

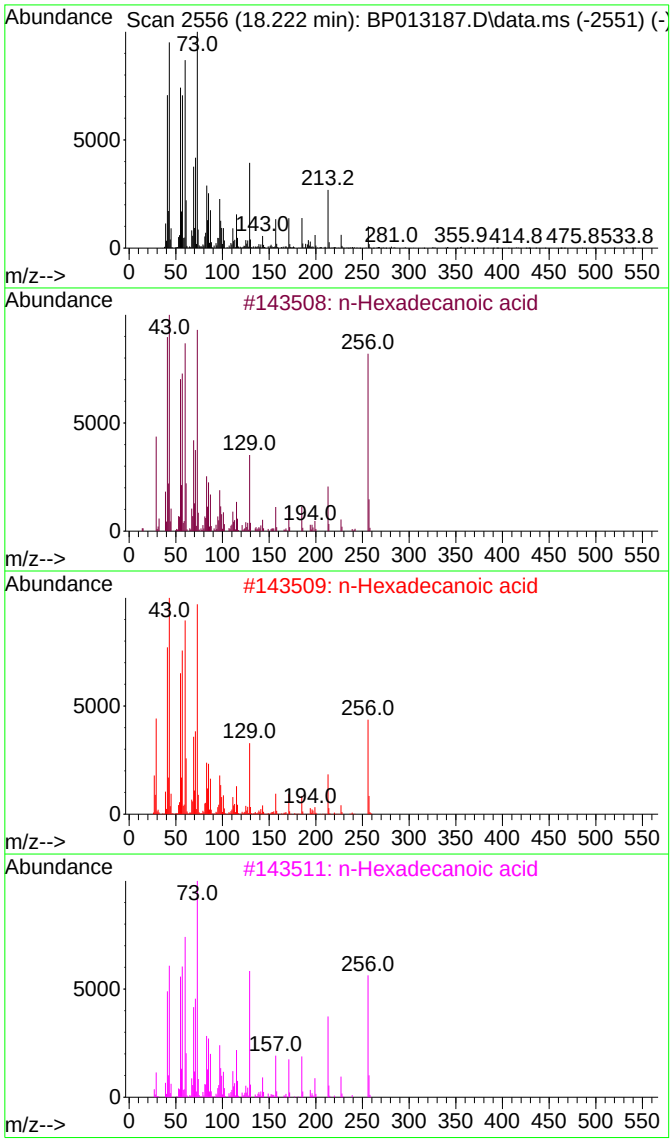
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

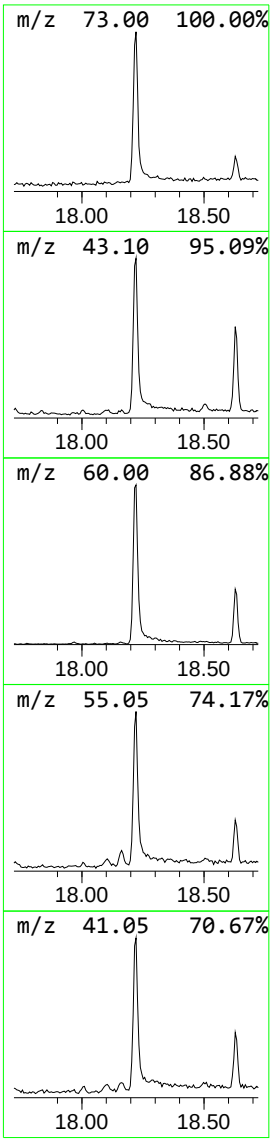
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	3.04 ng/ul	790595	Phenanthrene-d10	17.351

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	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	Octadecanoic acid	284	C18H36O2	000057-11-4	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013187.D
Acq On : 21 Dec 2022 03:18
Operator : CG/JU
Sample : N6009-04
Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB6

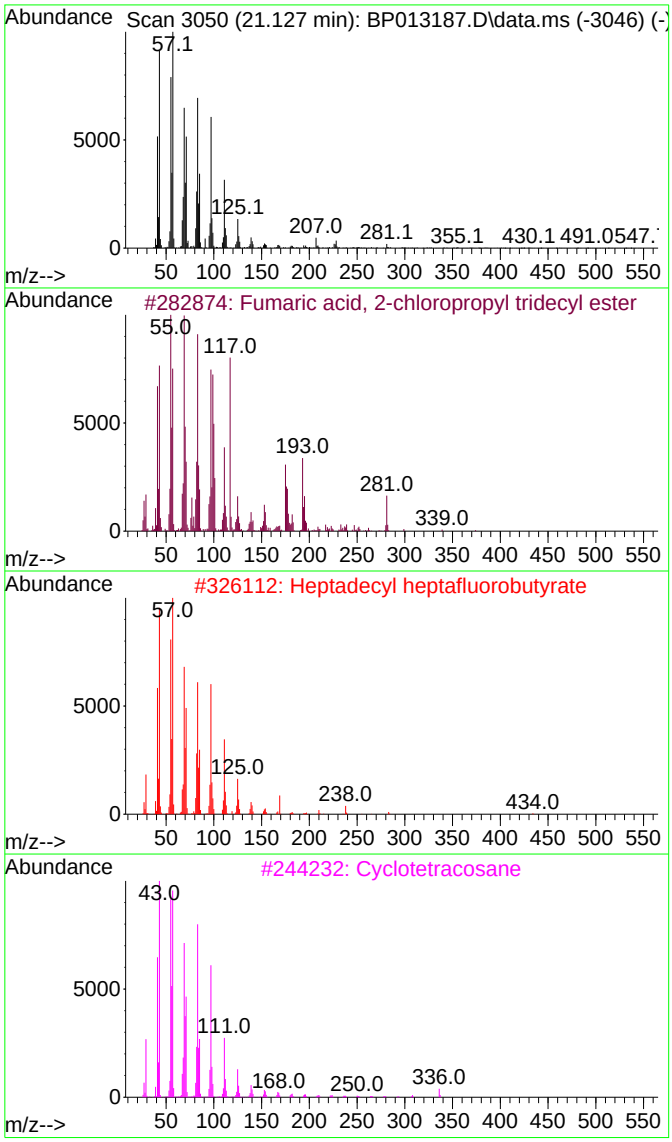
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

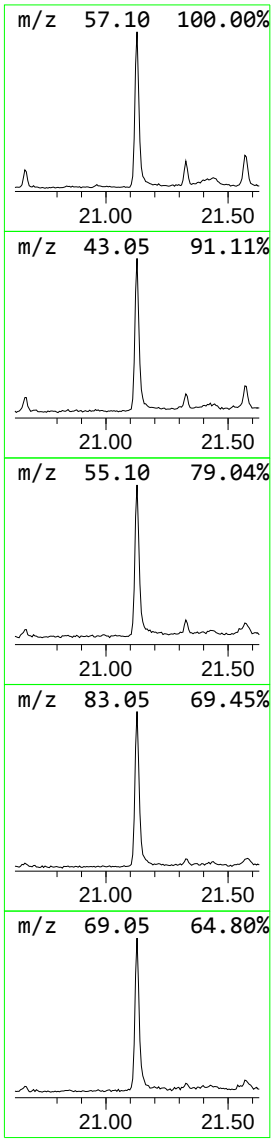
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Fumaric acid, 2-chloropropy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	4.75 ng/ul	1527200	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1010348-57-1	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Cyclotetracosane	336	C24H48	000297-03-0	94
4	1-Hexacosene	364	C26H52	018835-33-1	94
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013187.D
Acq On : 21 Dec 2022 03:18
Operator : CG/JU
Sample : N6009-04
Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB6

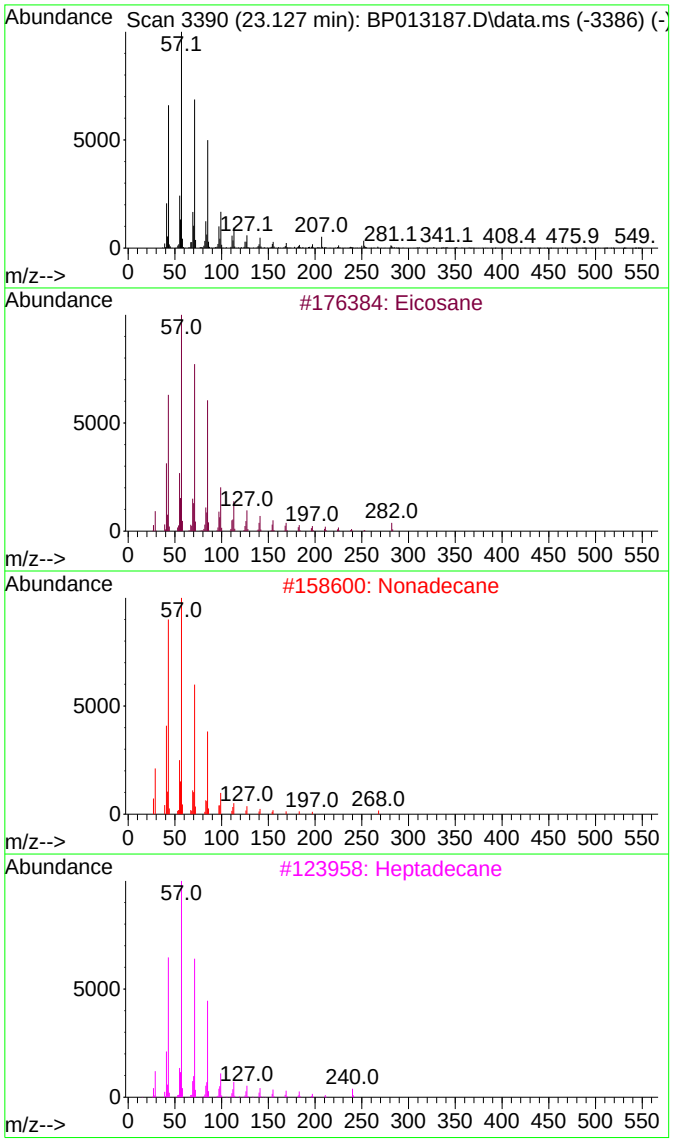
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

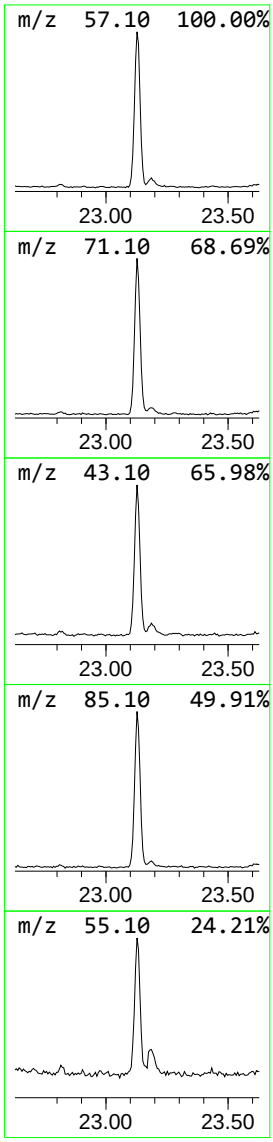
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.127	4.06 ng/ul	1454610	Perylene-d12	23.915

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	96
2	Nonadecane	268	C19H40	000629-92-5	94
3	Heptadecane	240	C17H36	000629-78-7	93
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
5	Eicosane, 9-octyl-	394	C28H58	013475-77-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013187.D
Acq On : 21 Dec 2022 03:18
Operator : CG/JU
Sample : N6009-04
Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB6

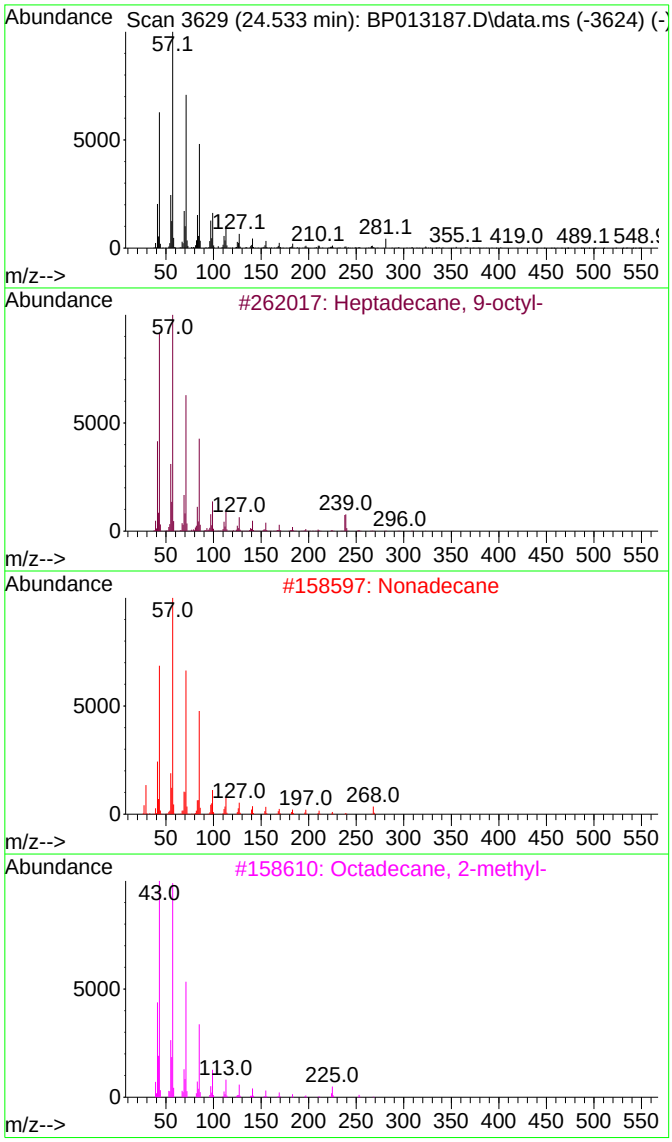
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

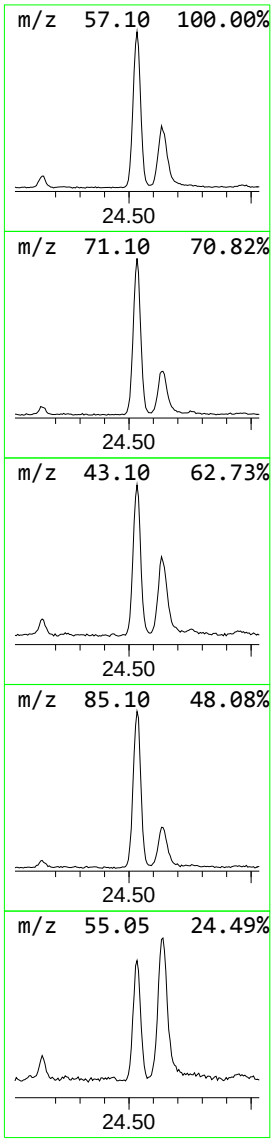
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.533	4.90 ng/ul	1753120	Perylene-d12	23.915

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2	Nonadecane	268	C19H40	000629-92-5	93
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
4	Tetracosane	338	C24H50	000646-31-1	90
5	Tetratetracontane	619	C44H90	007098-22-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013187.D
Acq On : 21 Dec 2022 03:18
Operator : CG/JU
Sample : N6009-04
Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB6

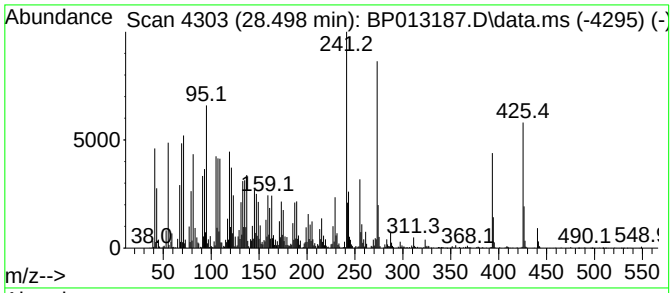
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

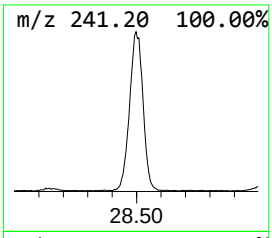
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

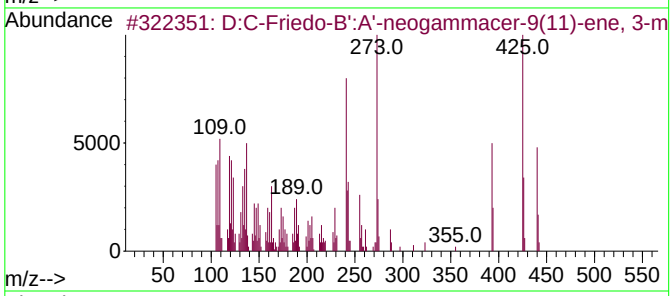
****
Peak Number 9 D:C-Friedo-B':A'-neogammace... Concentration Rank 1

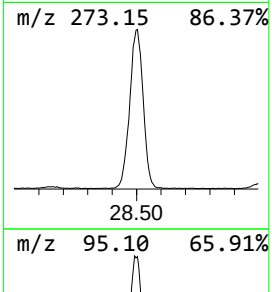
R.T.	EstConc	Area	Relative to ISTD	R.T.
28.498	29.95 ng/ul	10719000	Perylene-d12	23.915

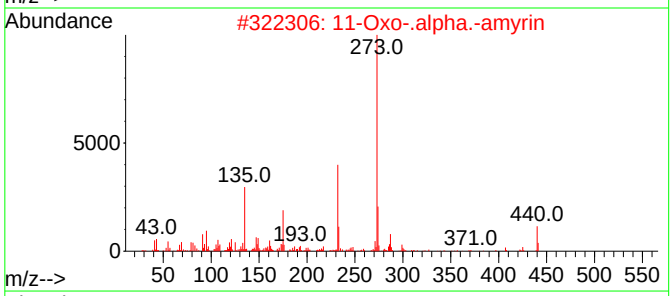
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	50
2	11-Oxo-.alpha.-amyrin	440	C30H48O2	002118-90-3	45
3	Benzene, 1-[2-(2-chloroethoxy)et...	312	C18H29ClO2	065925-28-2	25
4	Indole, 5-chloro-2-methyl-3-phenyl-	241	C15H12ClN	030843-37-9	25
5	2-Amino-.alpha.-[2-chlorophenyl]...	273	C15H12ClNO2	1000254-08-5	25

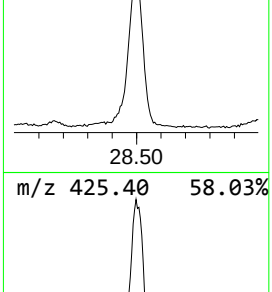


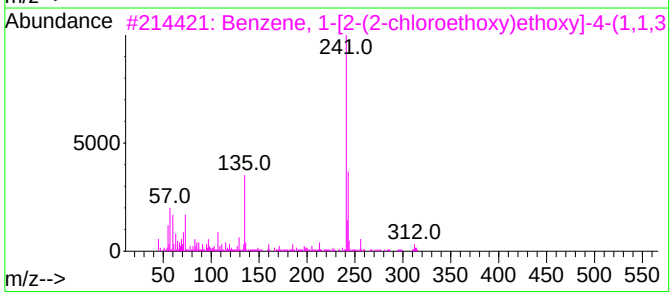


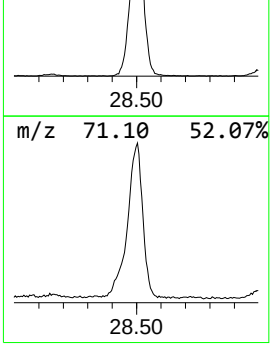












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013187.D
Acq On : 21 Dec 2022 03:18
Operator : CG/JU
Sample : N6009-04
Misc :
ALS Vial : 69 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYB6

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
(1R)-2,6,6-Trim...	6.622	5.9	ng/ul	767964	1	7.952	2585170	20.0
.beta.-Pinene	7.387	2.4	ng/ul	312924	1	7.952	2585170	20.0
Benzophenone	15.951	2.4	ng/ul	551529	3	14.592	4546230	20.0
n-Hexadecanoic ...	18.222	3.0	ng/ul	790595	4	17.351	5196630	20.0
Fumaric acid, 2...	21.127	4.8	ng/ul	1527200	5	21.433	6429380	20.0
(DEL) Alkane: S...	23.127	4.1	ng/ul	1454610	6	23.915	7156980	20.0
(DEL) Alkane: S...	24.533	4.9	ng/ul	1753120	6	23.915	7156980	20.0
D:C-Friedo-B':A...	28.498	29.9	ng/ul	10719000	6	23.915	7156980	20.0