LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138179.D
Acq On : 10 Jun 2024 18:38
Operator : CG\JU
Sample : P2794-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-060724

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_F\Methods\8270-BF060524.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138179.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	8	14	19	rBV	2373267	2938780	69.00%	4.733%
2	5.104	510	513	518	rVB	171921	176151	4.14%	0.284%
3	5.504	577	581	585	rBV	3761133	3428429	80.50%	5.522%
4	6.510	748	752	755	rBV	3686746	3482347	81.76%	5.609%
5	6.893	814	817	821	rBV	2420569	2062330	48.42%	3.322%
6	7.451	908	912	915	rBV	2434758	1934030	45.41%	3.115%
7	8.175	1032	1035	1038	rBV	3315226	2663096	62.53%	4.289%
8	8.987	1169	1173	1177	rBV	70681	67066	1.57%	0.108%
9	9.251	1214	1218	1221	rBV	5785963	4258984	100.00%	6.860%
10	9.586	1270	1275	1277	rBV	66698	65728	1.54%	0.106%
11	9.792	1306	1310	1314	rBV	54931	57029	1.34%	0.092%
12	9.928	1330	1333	1337	rVV	3140316	2684047	63.02%	4.323%
13	9.963	1337	1339	1342	rVB	95663	71290	1.67%	0.115%
14	10.134	1364	1368	1372	rVB	63291	63686	1.50%	0.103%
15	10.475	1423	1426	1431	rVB	110134	99616	2.34%	0.160%
16	10.716	1463	1467	1471	rBV	2021291	1602922	37.64%	2.582%
17	10.833	1484	1487	1495	rVB3	119333	158379	3.72%	0.255%
18	11.022	1513	1519	1522	rBV3	69653	86717	2.04%	0.140%
19	11.280	1557	1563	1566	rBV2	118045	135146	3.17%	0.218%
20	11.310	1566	1568	1573	rVB	117967	114206	2.68%	0.184%
21	11.416	1582	1586	1588	rBV	2824891	2213407	51.97%	3.565%
22	11.439	1588	1590	1593	rVV	1462175	1065469	25.02%	1.716%
23	11.492	1593	1599	1601	rVB	226976	222366	5.22%	0.358%
24	11.645	1619	1625	1627	rBV	74795	90573	2.13%	0.146%
25	11.710	1633	1636	1640	rBV2	125417	102727	2.41%	0.165%
26	11.810	1650	1653	1660	rVB	643059	518960	12.19%	0.836%
27	11.916	1668	1671	1673	rBV	232855	183457	4.31%	0.295%
28	11.945	1673	1676	1679	rVB2	387271	367150	8.62%	0.591%
29	12.028	1687	1690	1692	rBV2	310862	297494	6.99%	0.479%
30	12.051	1692	1694	1699	rVB	182751	146477	3.44%	0.236%
31	12.116	1699	1705	1708	rBV	105622	119505	2.81%	0.192%
32	12.210	1719	1721	1723	rBV	147253	135671	3.19%	0.219%
33	12.233	1723	1725	1732	rVB2	129561	128851	3.03%	0.208%
34	12.392	1749	1752	1754	rBV	75802	63271	1.49%	0.102%
35	12.463	1761	1764	1767	rBV	159416	168330	3.95%	0.271%
36	12.498	1767	1770	1772	rVV	3039522	2562125	60.16%	4.127%

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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-04-060724

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_F\Methods\8270-BF060524.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.522	1772	1774	1777	rVV	1762183	1577334	37.04%	2.540%
38	12.545	1777	1778	1783	rVV2	193863	173761	4.08%	0.280%
39	12.604	1785	1788	1789	rVV	321362	253079	5.94%	0.408%
40	12.627	1789	1792	1796	rVB	3337532	2640844	62.01%	4.253%
41	12.722	1805	1808	1810	rBV3	91130	76700	1.80%	0.124%
42	12.780	1815	1818	1821	rVV	107801	93828	2.20%	0.151%
43	12.857	1825	1831	1834	rBV	3002201	2833604	66.53%	4.564%
44	12.904	1837	1839	1844	rVB2	109493	128291	3.01%	0.207%
45	12.975	1848	1851	1852	rBV	146743	118391	2.78%	0.191%
46	12.998	1852	1855	1863	rVB	3942130	3478236	81.67%	5.602%
47	13.074	1863	1868	1871	rBV3	174045	282835	6.64%	0.456%
48	13.163	1880	1883	1884	rBV3	127994	149358	3.51%	0.241%
49	13.180	1884	1886	1890	rVB	284145	275683	6.47%	0.444%
50	13.251	1893	1898	1900	rBV2	204449	204066	4.79%	0.329%
51	13.286	1900	1904	1907	rBV2	292545	281702	6.61%	0.454%
52	13.380	1917	1920	1922	rVB	154462	120835	2.84%	0.195%
53	13.410	1922	1925	1929	rBV	163044	146565	3.44%	0.236%
54	13.480	1934	1937	1942	rVB	174528	170371	4.00%	0.274%
55	13.580	1951	1954	1957	rBV3	74568	76175	1.79%	0.123%
56	13.686	1969	1972	1978	rVB	283120	266394	6.25%	0.429%
57	13.804	1987	1992	1994	rBV2	271335	355882	8.36%	0.573%
58	13.833	1994	1997	1998	rVV	207096	173115	4.06%	0.279%
59	13.851	1998	2000	2005	rVV2	190448	256039	6.01%	0.412%
60	13.892	2005	2007	2012	rVB3	187945	246572	5.79%	0.397%
61	14.051	2029	2034	2037	rBV2	2951259	3940742	92.53%	6.347%
62	14.080	2037	2039	2045	rVB	1518309	1270222	29.82%	2.046%
63	14.157	2050	2052	2055	rVB	173173	131444	3.09%	0.212%
64	14.192	2056	2058	2060	rBV	61828	66159	1.55%	0.107%
65	14.263	2068	2070	2076	rVB2	151418	170507	4.00%	0.275%
66	14.404	2091	2094	2095	rBV	91461	84026	1.97%	0.135%
67	14.439	2095	2100	2103	rVB	224270	283317	6.65%	0.456%
68	14.474	2103	2106	2109	rVB	127682	116817	2.74%	0.188%
69	14.527	2113	2115	2118	rVB2	177525	156165	3.67%	0.252%
70	14.563	2118	2121	2123	rBV	132498	134083	3.15%	0.216%
71	14.916	2178	2181	2187	rBV2	216888	283992	6.67%	0.457%
72	14.992	2191	2194	2199	rVB3	111214	163815	3.85%	0.264%
73	15.098	2207	2212	2215	rBV	1003314	1568598	36.83%	2.526%
74	15.404	2260	2264	2270	rVB	627011	765901	17.98%	1.234%
75	15.463	2270	2274	2279	rBV	765356	929951	21.84%	1.498%
76	15.527	2281	2285	2289	rVV	1157480	1507491	35.40%	2.428%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
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Acq On : 10 Jun 2024 18:38
Operator : CG\JU
Sample : P2794-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-060724

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_F\Methods\8270-BF060524.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	15.563	2289	2291	2298	rVB2	249750	359047	8.43%	0.578%
78	16.027	2367	2370	2374	rBV	103419	130029	3.05%	0.209%
79	17.010	2532	2537	2546	rVB2	304514	641436	15.06%	1.033%
80	17.457	2608	2613	2622	rVB	243211	468853	11.01%	0.755%

Sum of corrected areas: 62088067

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
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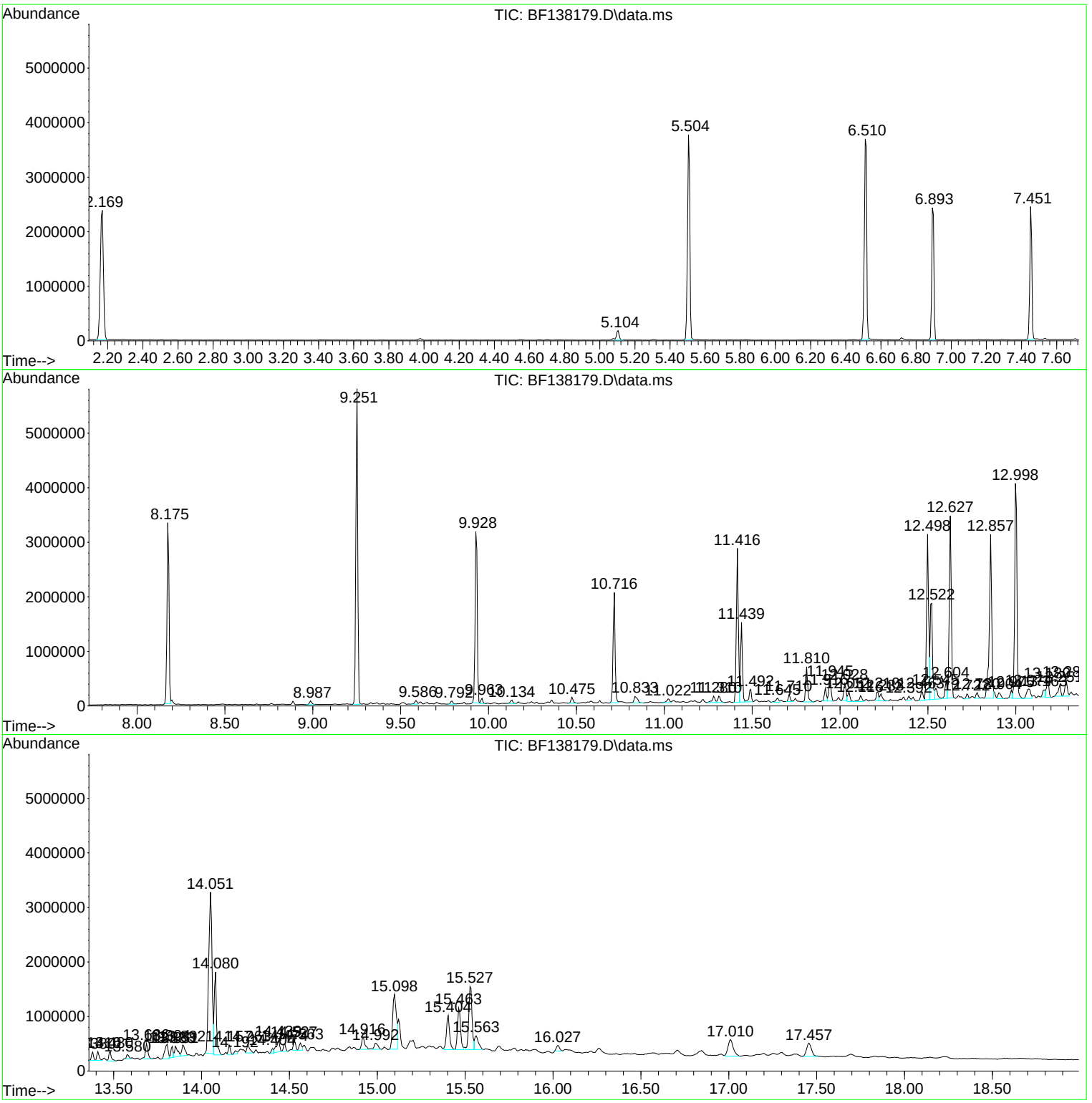
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-060724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

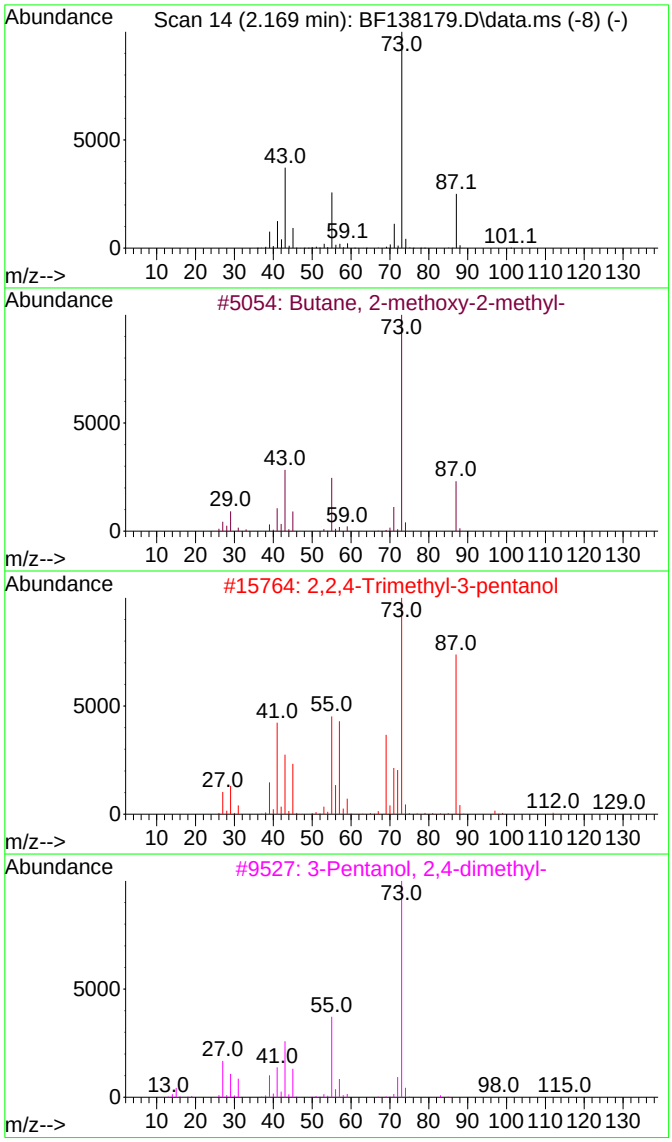
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

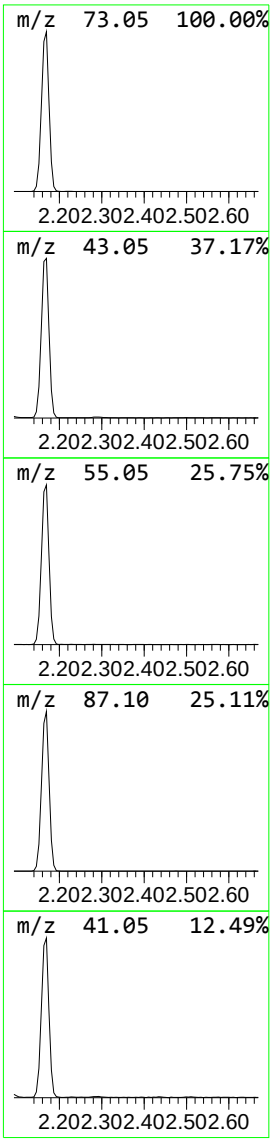
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	28.50 ng	2938780	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Instrument :
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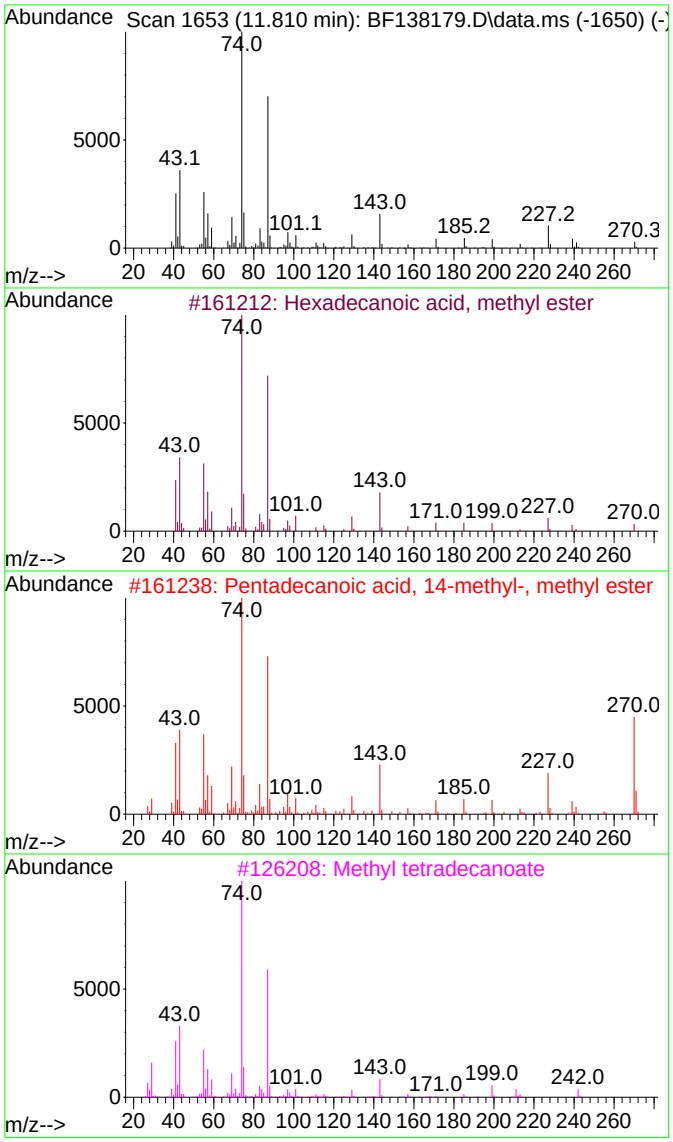
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

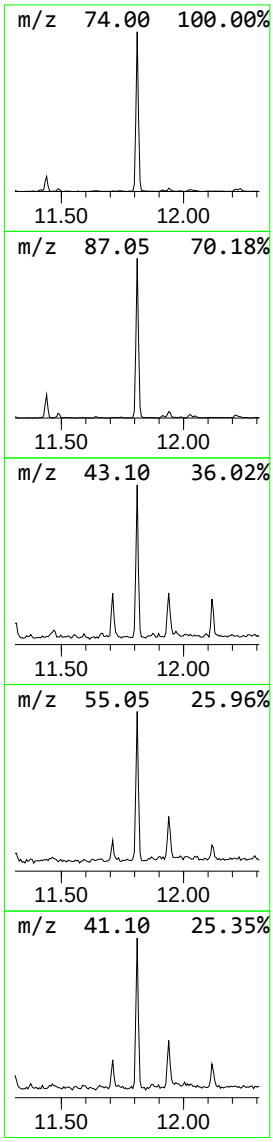
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	4.69 ng	518960	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	89
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





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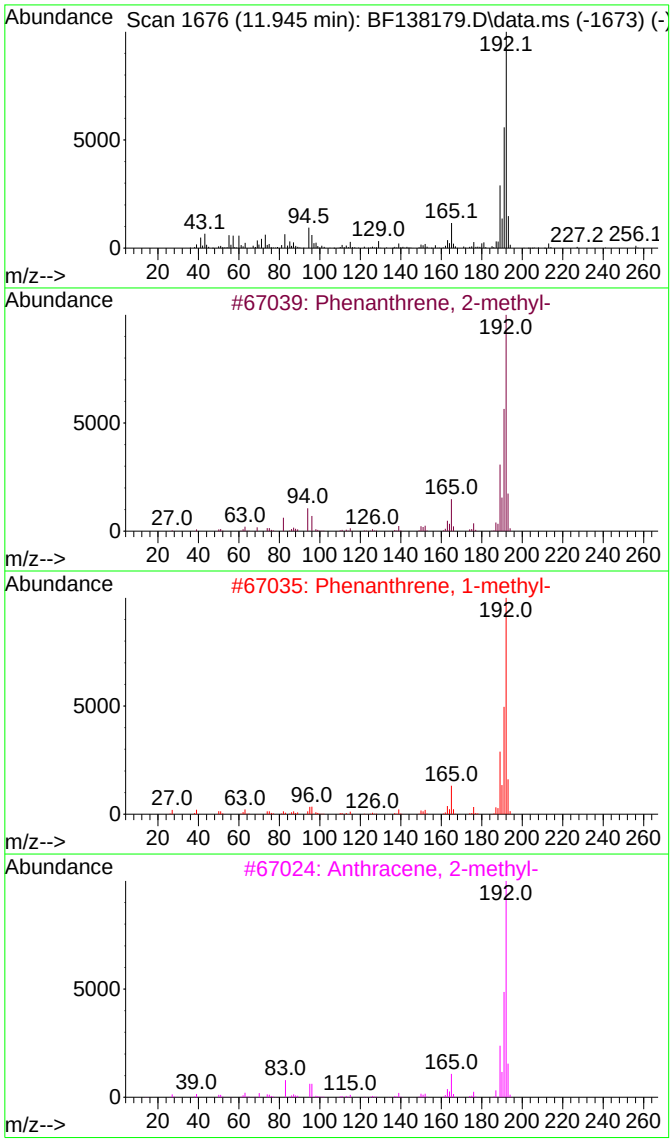
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

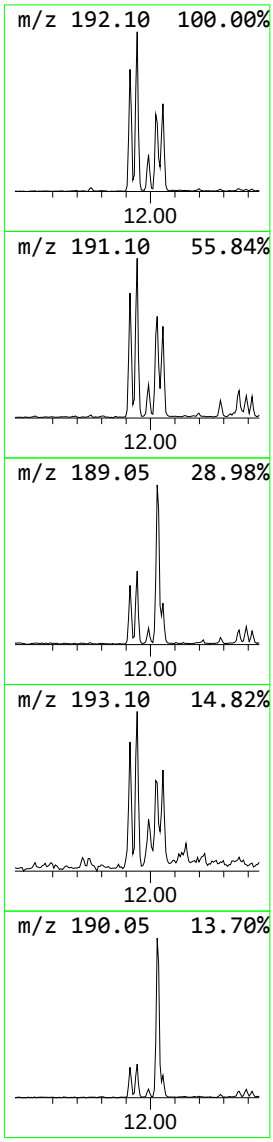
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	3.32 ng	367150	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	98
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	95
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	94





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BNA_F
ClientSampleId :
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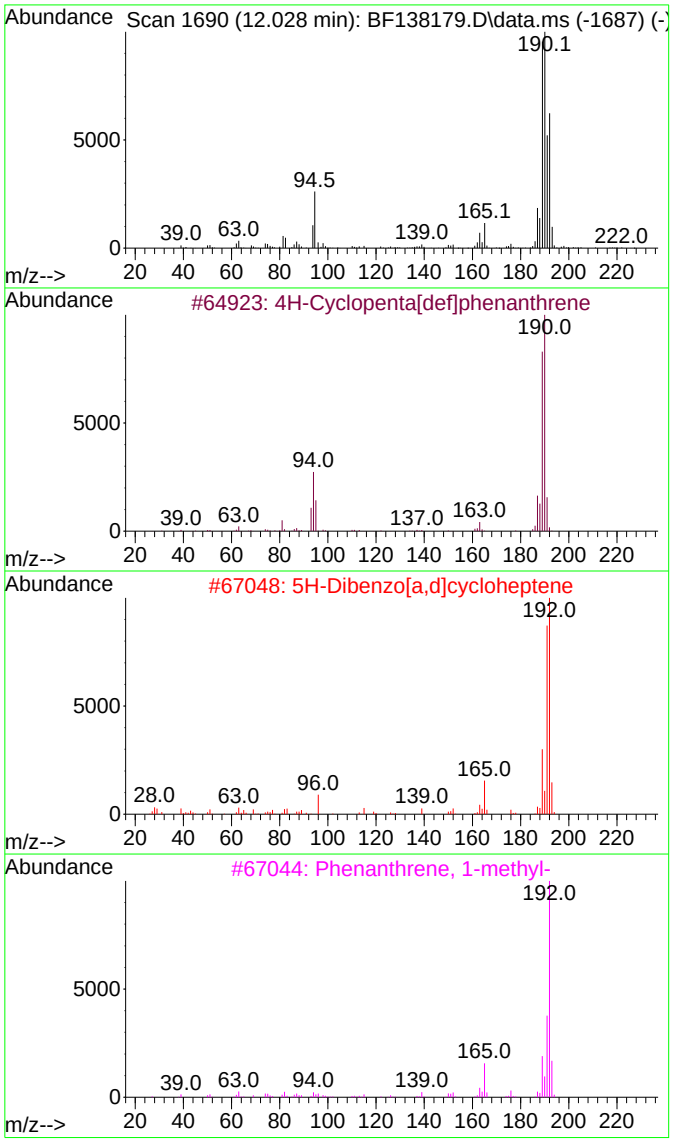
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

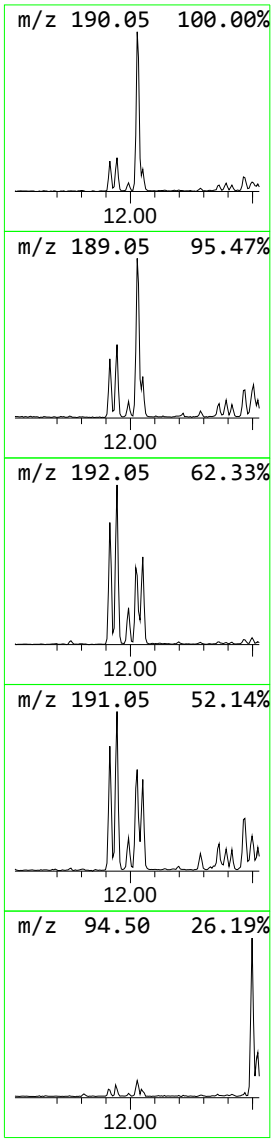
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.028	2.69 ng	297494	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	38
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	35
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	35
5	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	25





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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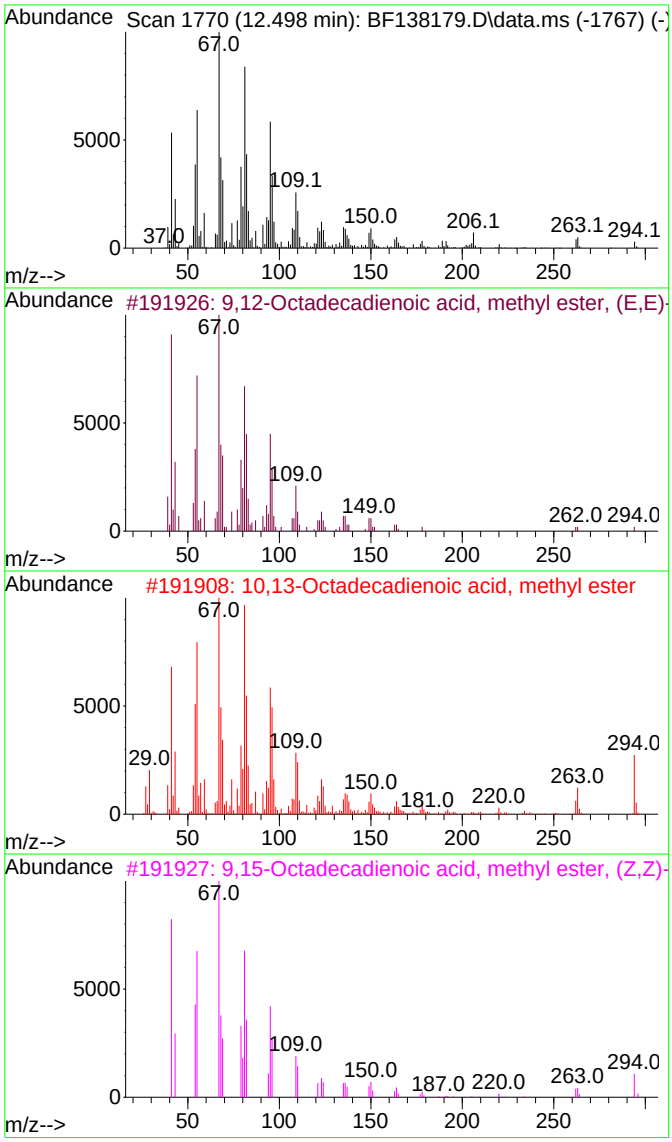
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

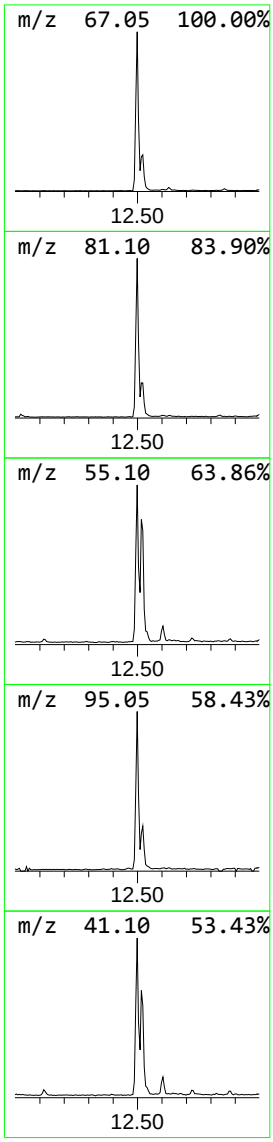
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.498	23.15 ng	2562130	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99





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Sample : P2794-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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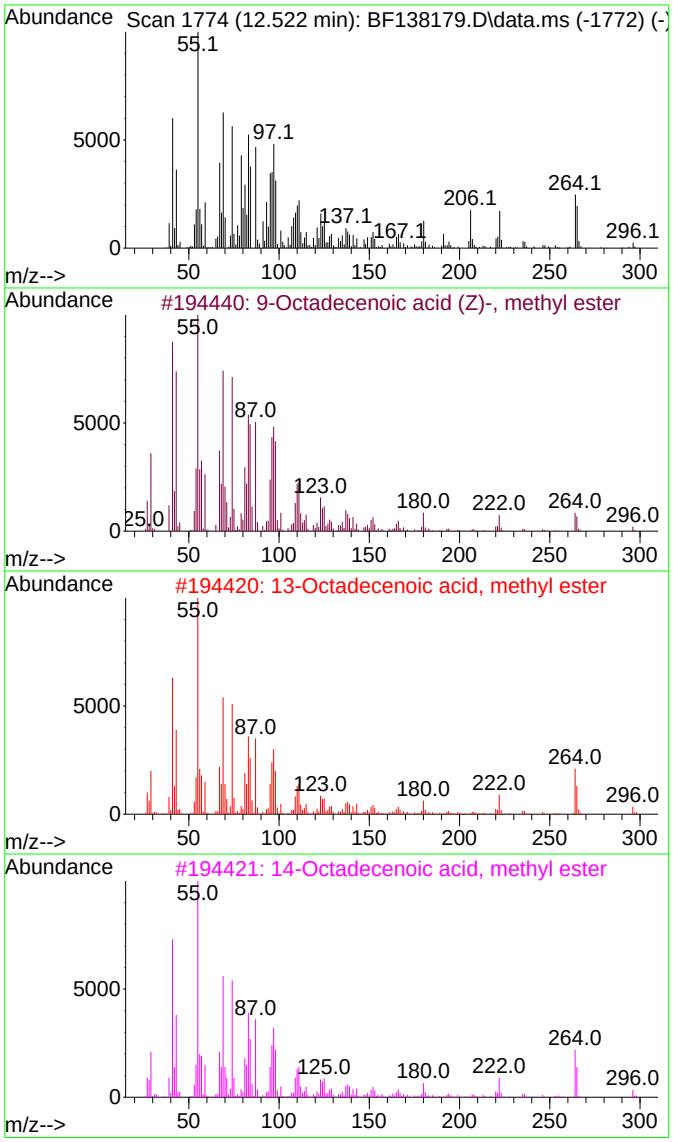
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

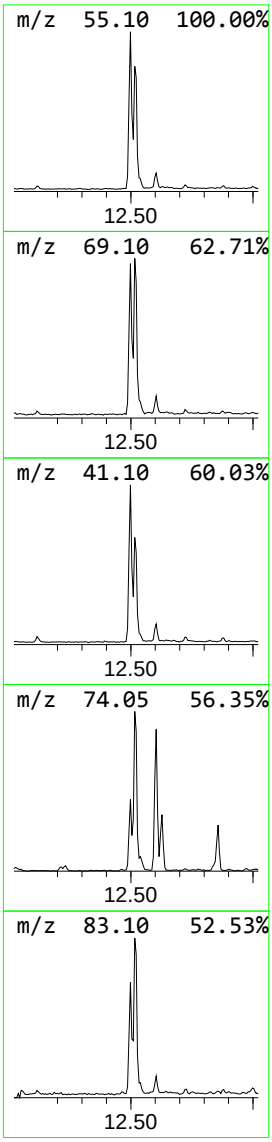
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.522	14.25 ng	1577330	Phenanthrene-d10	11.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	98
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	98





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Data File : BF138179.D
Acq On : 10 Jun 2024 18:38
Operator : CG\JU
Sample : P2794-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-060724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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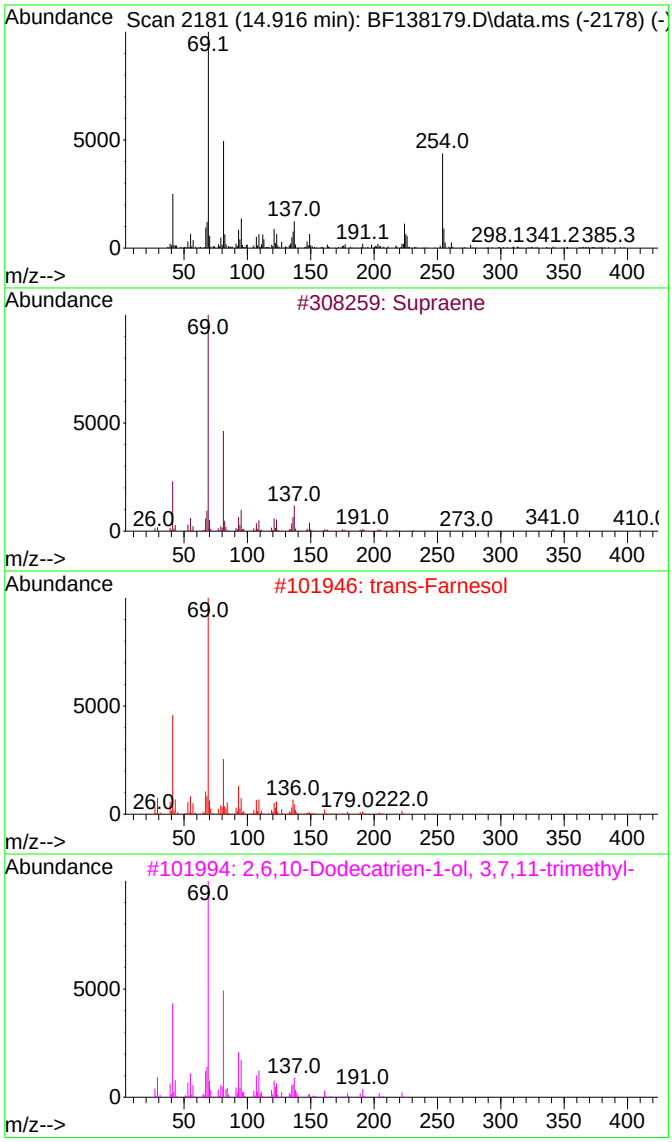
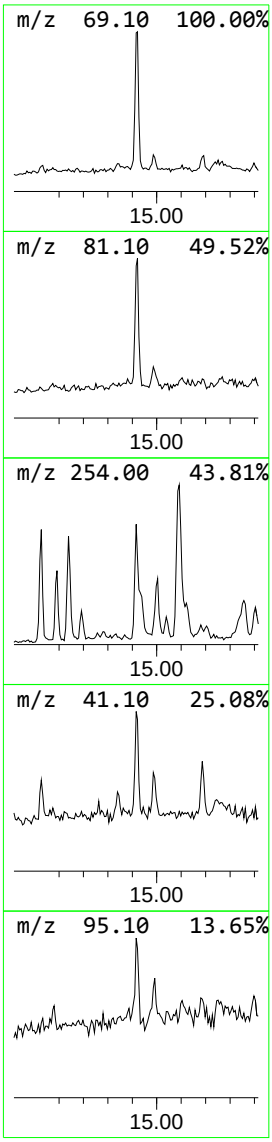
Peak Number 7 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.916	3.77 ng	283992	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	55
2	trans-Farnesol	222	C15H26O	000106-28-5	50
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	46
4	Squalene	410	C30H50	000111-02-4	43
5	Farnesol isomer a	222	C15H26O	1000108-92-4	43





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Data File : BF138179.D
Acq On : 10 Jun 2024 18:38
Operator : CG\JU
Sample : P2794-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-060724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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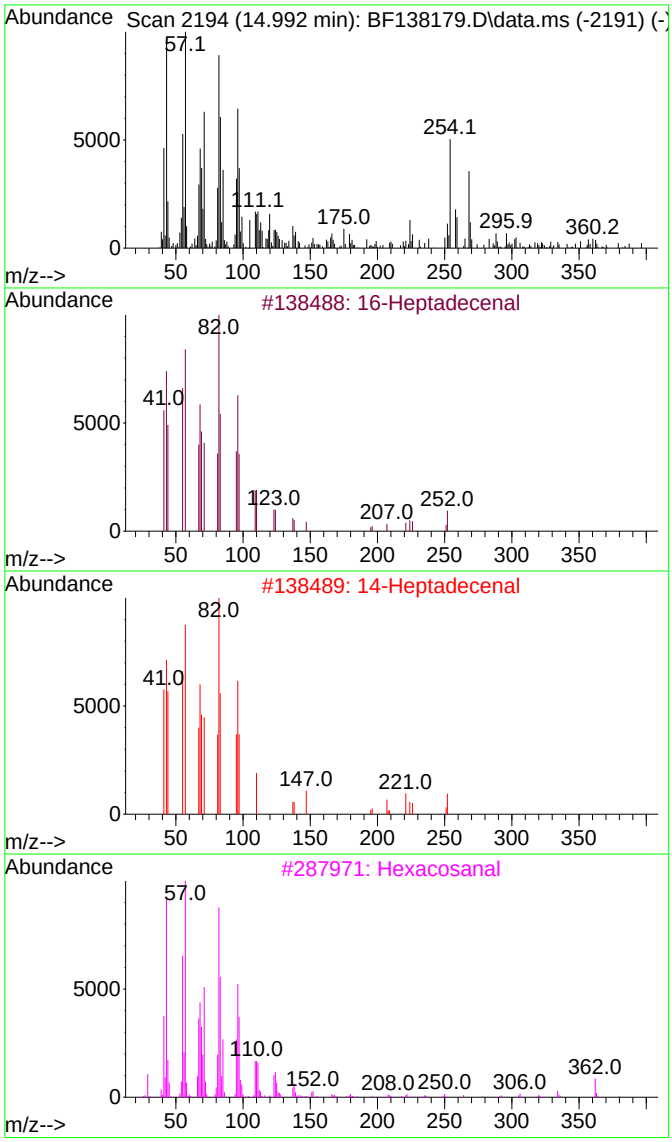
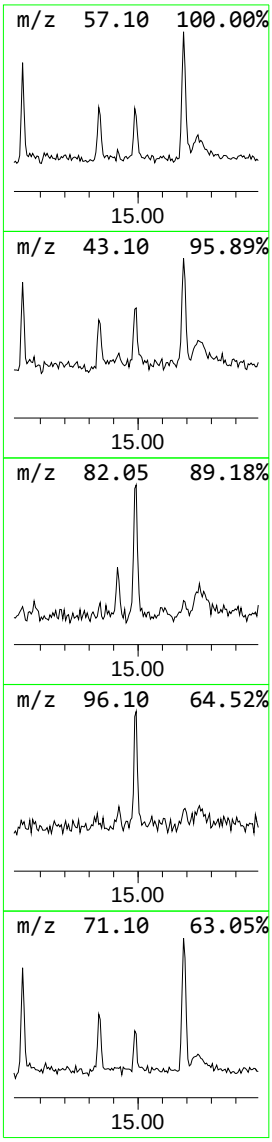
Peak Number 8 16-Heptadecenal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.992	2.17 ng	163815	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Heptadecenal	252	C17H32O	1010144-57-9	91
2	14-Heptadecenal	252	C17H32O	1010144-58-0	64
3	Hexacosanal	380	C26H52O	026627-85-0	60
4	Octadecanal	268	C18H36O	000638-66-4	53
5	1,19-Eicosadiene	278	C20H38	014811-95-1	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138179.D
Acq On : 10 Jun 2024 18:38
Operator : CG\JU
Sample : P2794-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-060724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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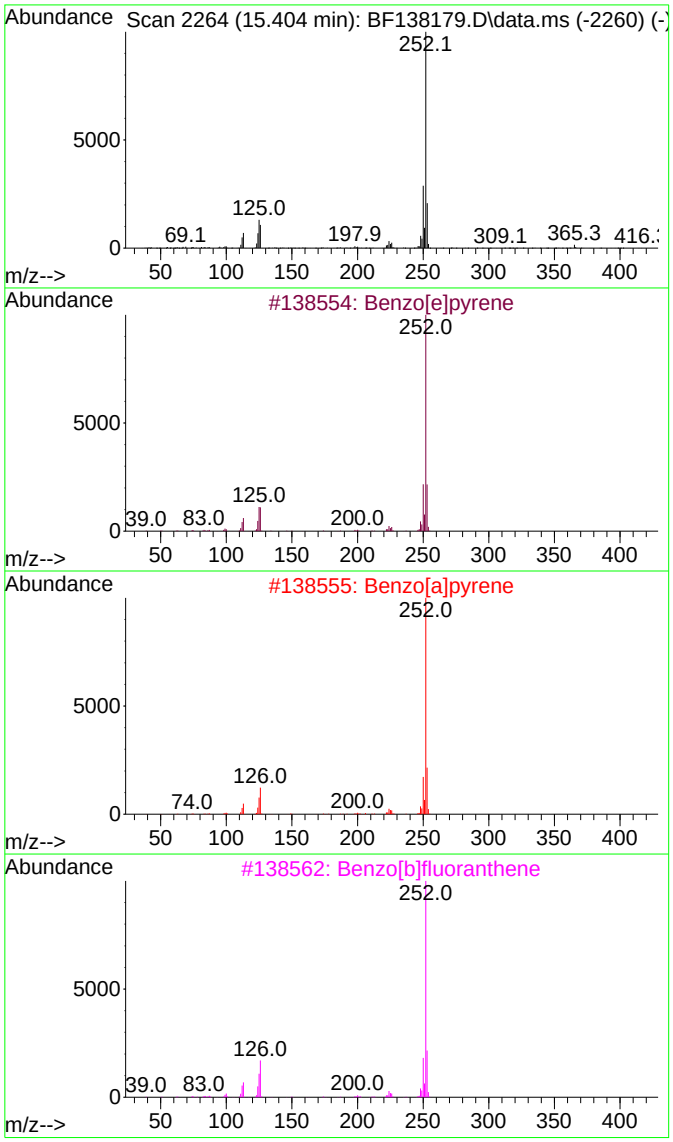
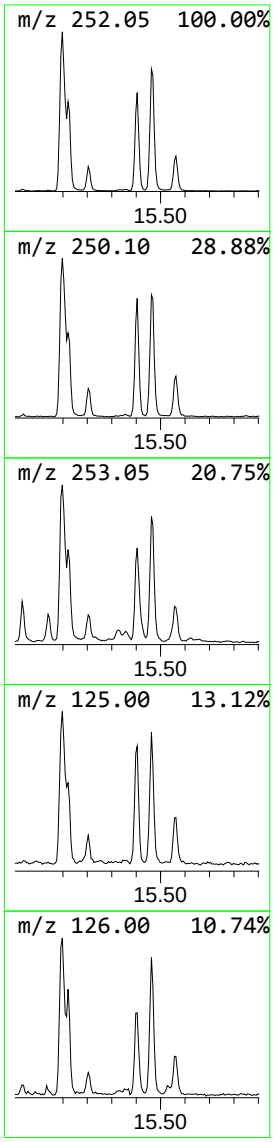
Peak Number 9 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	10.16 ng	765901	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
5	Perylene	252	C20H12	000198-55-0	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061024\
Data File : BF138179.D
Acq On : 10 Jun 2024 18:38
Operator : CG\JU
Sample : P2794-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-060724

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
Butane, 2-metho...	2.169	28.5	ng	2938780	1	6.898	2062330	20.0
Hexadecanoic ac...	11.810	4.7	ng	518960	4	11.416	2213410	20.0
Phenanthrene, 2...	11.945	3.3	ng	367150	4	11.416	2213410	20.0
4H-Cyclopenta[d...	12.028	2.7	ng	297494	4	11.416	2213410	20.0
9,12-Octadecadi...	12.498	23.1	ng	2562130	4	11.416	2213410	20.0
9-Octadecenoic ...	12.522	14.3	ng	1577330	4	11.416	2213410	20.0
Supraene	14.916	3.8	ng	283992	6	15.527	1507490	20.0
16-Heptadecenal	14.992	2.2	ng	163815	6	15.527	1507490	20.0
Benzo[e]pyrene	15.404	10.2	ng	765901	6	15.527	1507490	20.0