LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138377.D
Acq On : 27 Jun 2024 20:39
Operator : CG\JU
Sample : P3077-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-N-1

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138377.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	20	rVB	2010106	2502117	80.29%	7.104%
2	2.275	28	32	37	rBV	28209	38976	1.25%	0.111%
3	3.399	219	223	232	rBV	81869	162472	5.21%	0.461%
4	3.475	232	236	252	rVB	16706	53751	1.72%	0.153%
5	5.099	508	512	519	rVB	232222	257668	8.27%	0.732%
6	5.504	577	581	585	rBV	3171381	3116535	100.00%	8.849%
7	6.516	748	753	756	rBV	3452333	3024544	97.05%	8.587%
8	6.704	782	785	789	rBV2	71121	67857	2.18%	0.193%
9	6.881	811	815	818	rVB	1607472	1259421	40.41%	3.576%
10	7.440	906	910	913	rBV	2313426	1951840	62.63%	5.542%
11	7.693	949	953	959	rVB	121114	102748	3.30%	0.292%
12	8.157	1029	1032	1035	rVB	1771569	1467005	47.07%	4.165%
13	8.375	1063	1069	1074	rVB2	40106	44262	1.42%	0.126%
14	8.469	1082	1085	1088	rVB	201228	157725	5.06%	0.448%
15	8.745	1129	1132	1135	rVB	65253	45788	1.47%	0.130%
16	9.234	1211	1215	1218	rBV	3937497	3094809	99.30%	8.787%
17	9.310	1225	1228	1230	rBV	73153	55021	1.77%	0.156%
18	9.569	1268	1272	1274	rBV	46402	41865	1.34%	0.119%
19	9.839	1313	1318	1320	rVB2	45840	39816	1.28%	0.113%
20	9.910	1327	1330	1333	rBV	1705305	1387980	44.54%	3.941%
21	9.945	1333	1336	1339	rVB	83417	71631	2.30%	0.203%
22	10.010	1342	1347	1353	rVB2	100781	128712	4.13%	0.365%
23	10.116	1360	1365	1369	rVB2	55337	57151	1.83%	0.162%
24	10.457	1420	1423	1429	rVB	108825	94954	3.05%	0.270%
25	10.698	1460	1464	1471	rBV	1972058	1608384	51.61%	4.567%
26	10.810	1480	1483	1492	rVB5	56475	79236	2.54%	0.225%
27	11.004	1511	1516	1519	rBV2	36012	44132	1.42%	0.125%
28	11.257	1553	1559	1561	rBV3	28079	40307	1.29%	0.114%
29	11.292	1562	1565	1573	rVB	59739	60040	1.93%	0.170%
30	11.398	1579	1583	1585	rBV	1448653	1205509	38.68%	3.423%
31	11.422	1585	1587	1590	rVV	763550	566529	18.18%	1.608%
32	11.469	1592	1595	1598	rVB	186527	162846	5.23%	0.462%
33	11.898	1664	1668	1670	rBV	111904	106778	3.43%	0.303%
34	11.922	1670	1672	1676	rVV2	262508	259585	8.33%	0.737%
35	11.975	1678	1681	1684	rVV	63591	66333	2.13%	0.188%
36	12.010	1684	1687	1689	rVV	201816	201723	6.47%	0.573%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138377.D
Acq On : 27 Jun 2024 20:39
Operator : CG\JU
Sample : P3077-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-N-1

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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.033	1689	1691	1694	rVB	83924	69089	2.22%	0.196%
38	12.192	1715	1718	1720	rBV	73432	56939	1.83%	0.162%
39	12.445	1758	1761	1764	rBV	72285	76540	2.46%	0.217%
40	12.486	1764	1768	1770	rVV3	51206	65052	2.09%	0.185%
41	12.533	1773	1776	1781	rBV2	52576	62993	2.02%	0.179%
42	12.610	1785	1789	1792	rBV	1309935	1078586	34.61%	3.062%
43	12.704	1802	1805	1807	rBV	55508	51293	1.65%	0.146%
44	12.839	1822	1828	1833	rVV	1085796	1102157	35.36%	3.129%
45	12.886	1833	1836	1841	rVB2	51362	64380	2.07%	0.183%
46	12.980	1848	1852	1855	rVB	3189686	2620198	84.07%	7.439%
47	13.051	1860	1864	1868	rBV2	77240	123780	3.97%	0.351%
48	13.139	1876	1879	1881	rBV4	59426	71114	2.28%	0.202%
49	13.163	1881	1883	1887	rVB	204497	161381	5.18%	0.458%
50	13.227	1892	1894	1897	rVB	151036	129184	4.15%	0.367%
51	13.269	1897	1901	1904	rBV2	125980	127385	4.09%	0.362%
52	13.363	1914	1917	1919	rVB2	63793	51809	1.66%	0.147%
53	13.392	1919	1922	1925	rBV2	68360	67605	2.17%	0.192%
54	13.551	1945	1949	1950	rBV4	39865	43779	1.40%	0.124%
55	13.669	1967	1969	1974	rVB	71760	70704	2.27%	0.201%
56	13.780	1984	1988	1991	rBV3	89496	120220	3.86%	0.341%
57	13.810	1991	1993	1995	rVV	94661	81575	2.62%	0.232%
58	13.833	1995	1997	2001	rVV2	77080	107723	3.46%	0.306%
59	13.874	2001	2004	2013	rVB3	238914	282162	9.05%	0.801%
60	14.033	2026	2031	2034	rBV2	1602116	1861569	59.73%	5.285%
61	14.057	2034	2035	2041	rVB	519253	405226	13.00%	1.151%
62	14.139	2047	2049	2051	rVB	87634	60308	1.94%	0.171%
63	14.416	2094	2096	2099	rVB	85007	79929	2.56%	0.227%
64	14.451	2100	2102	2105	rVB2	55824	48943	1.57%	0.139%
65	14.510	2108	2112	2115	rBV3	62849	95071	3.05%	0.270%
66	14.545	2115	2118	2119	rBV	45055	38124	1.22%	0.108%
67	15.074	2204	2208	2211	rBV	326908	490321	15.73%	1.392%
68	15.180	2224	2226	2231	rVB	73506	73849	2.37%	0.210%
69	15.380	2256	2260	2266	rVB	162897	218183	7.00%	0.619%
70	15.439	2266	2270	2276	rVB	267654	318318	10.21%	0.904%
71	15.504	2276	2281	2285	rBV	764877	906462	29.09%	2.574%
72	16.968	2527	2530	2538	rVB2	95028	194603	6.24%	0.553%
73	17.421	2602	2607	2612	rVB	60985	118433	3.80%	0.336%

Sum of corrected areas: 35221037

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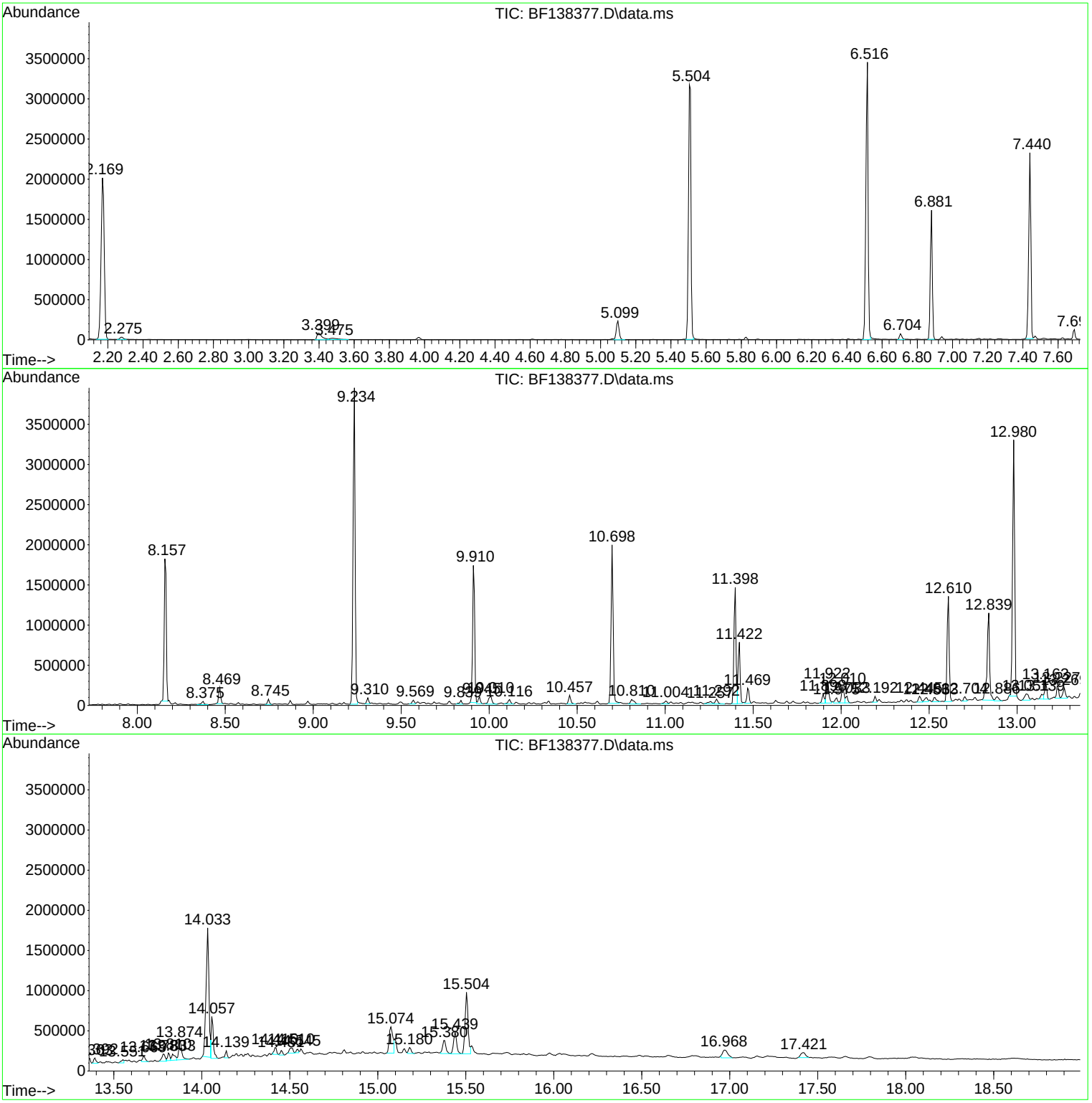
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-N-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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\BF062724\
Data File : BF138377.D
Acq On : 27 Jun 2024 20:39
Operator : CG\JU
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Instrument :
BNA_F
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1-N-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

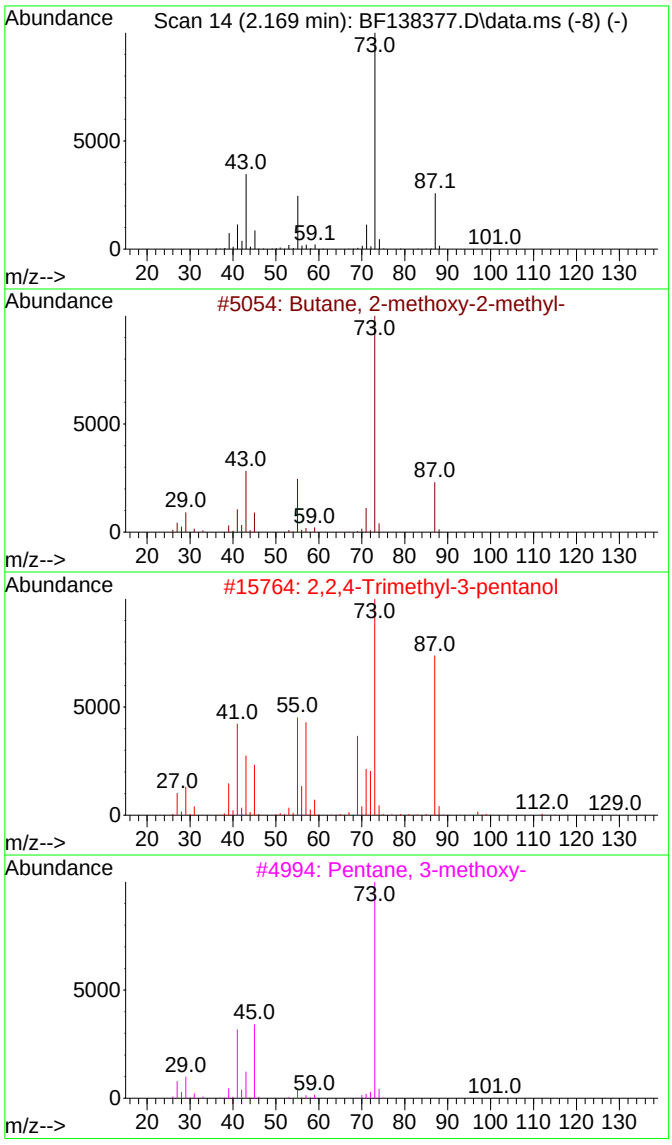
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

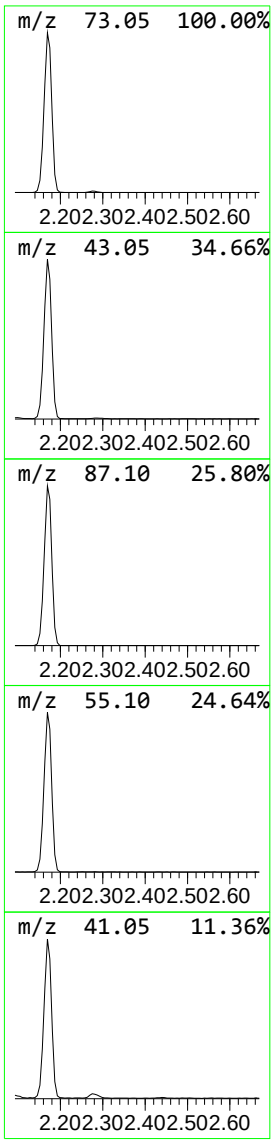
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	39.73 ng	2502120	1,4-Dichlorobenzene-d4	6.881

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	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138377.D
Acq On : 27 Jun 2024 20:39
Operator : CG\JU
Sample : P3077-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-N-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

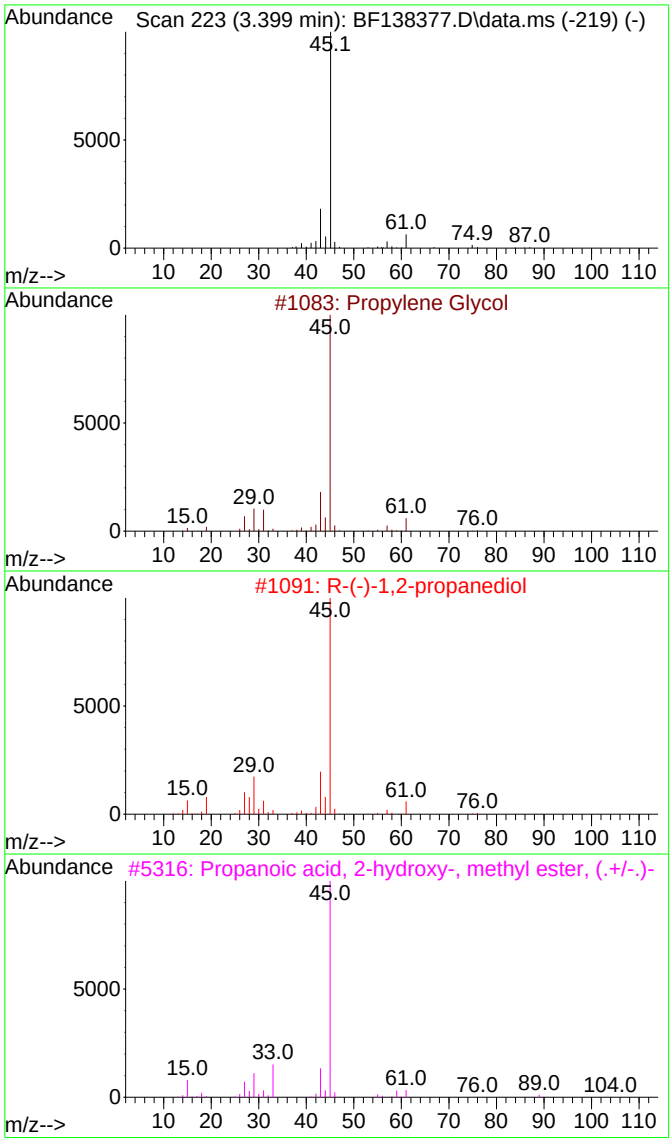
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

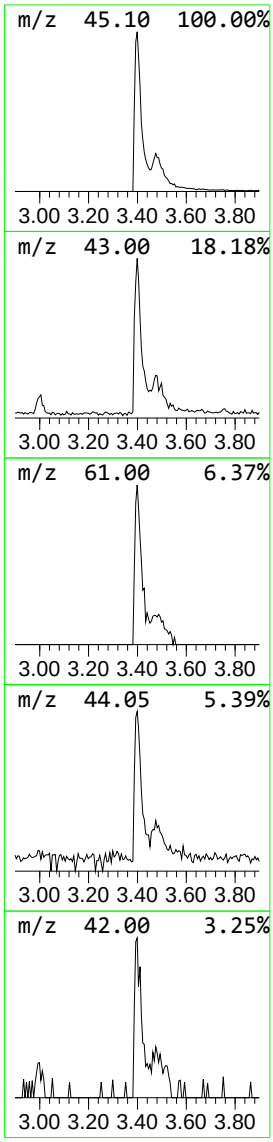
****

Peak Number 2 Propylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.399	2.58 ng	162472	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
4	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9
5	Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138377.D
Acq On : 27 Jun 2024 20:39
Operator : CG\JU
Sample : P3077-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-N-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

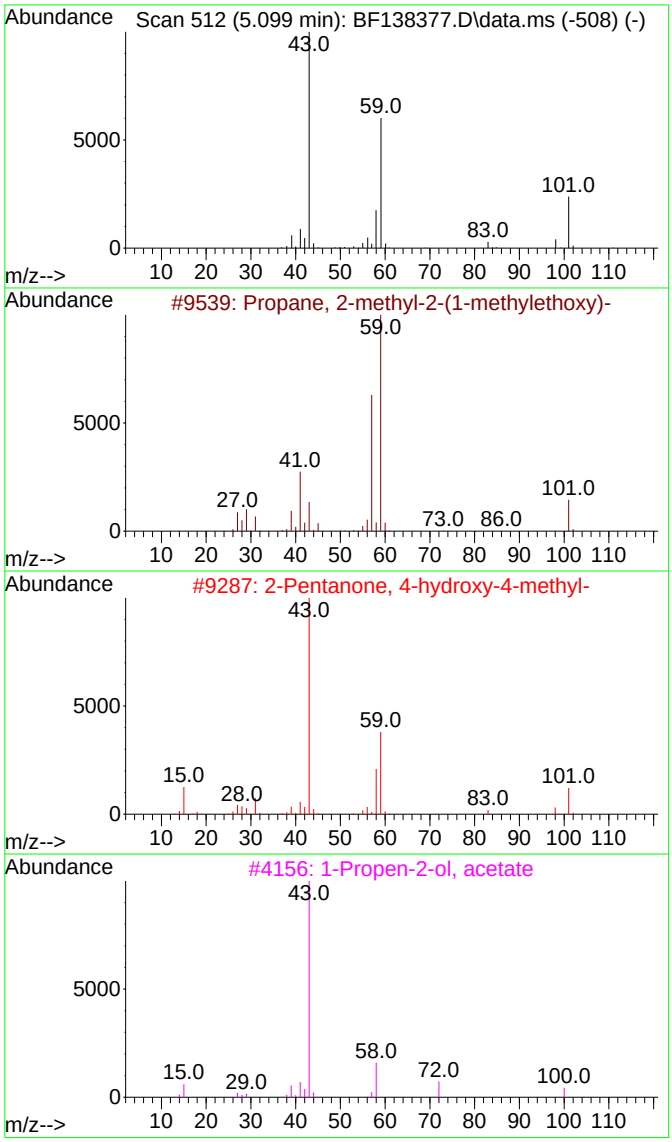
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

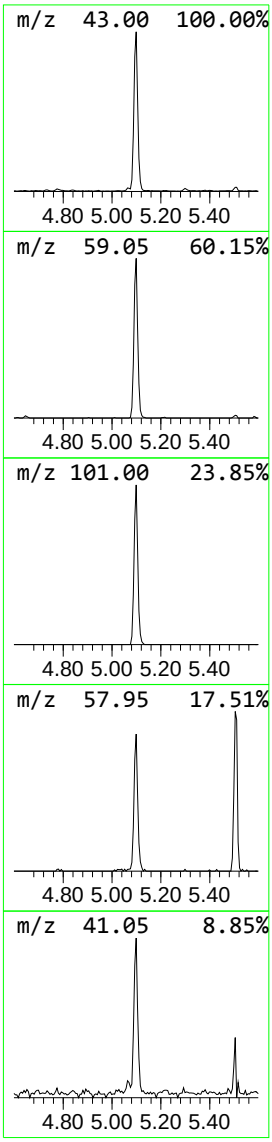
****

Peak Number 3 Propane, 2-methyl-2-(1-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	4.09 ng	257668	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138377.D
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

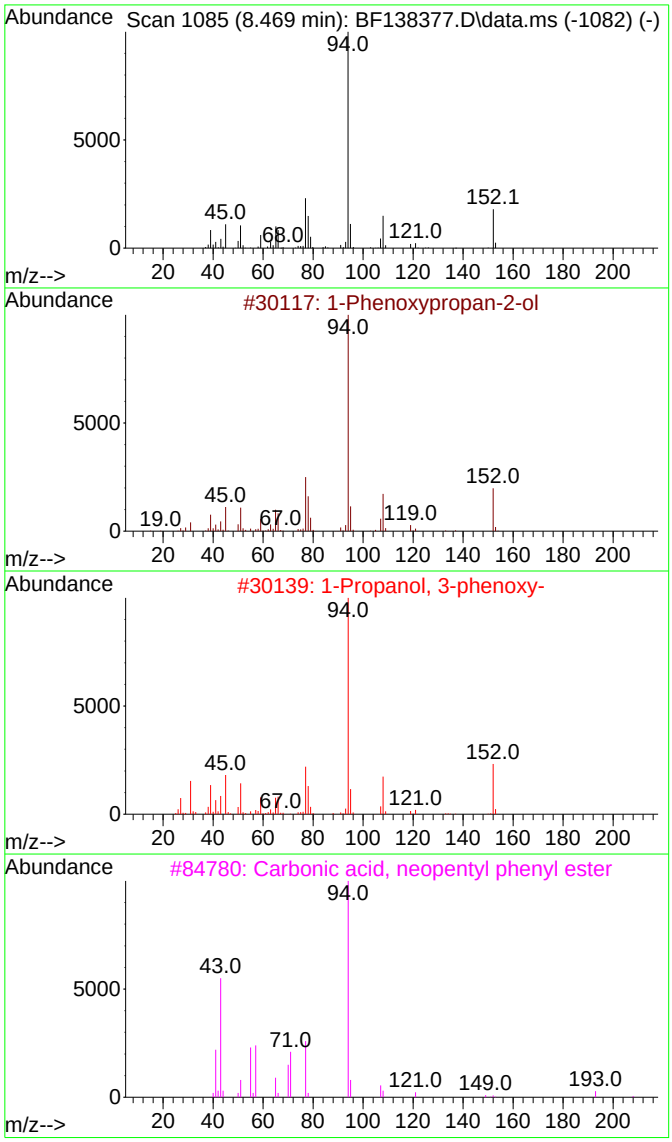
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

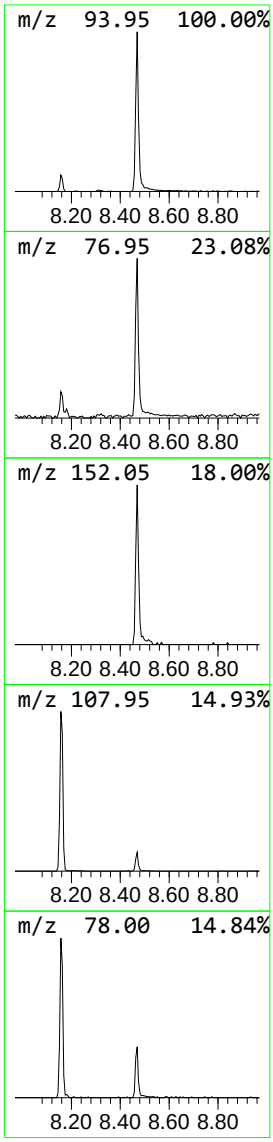
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	2.15 ng	157725	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	90
3	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138377.D
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Sample : P3077-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-N-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

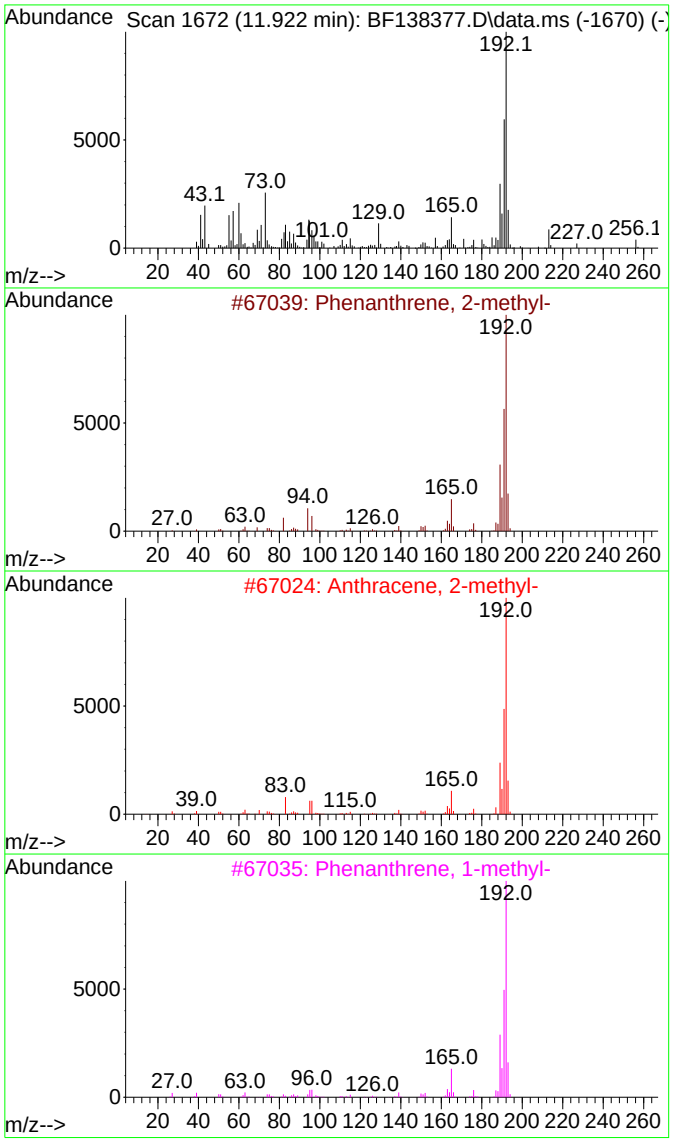
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

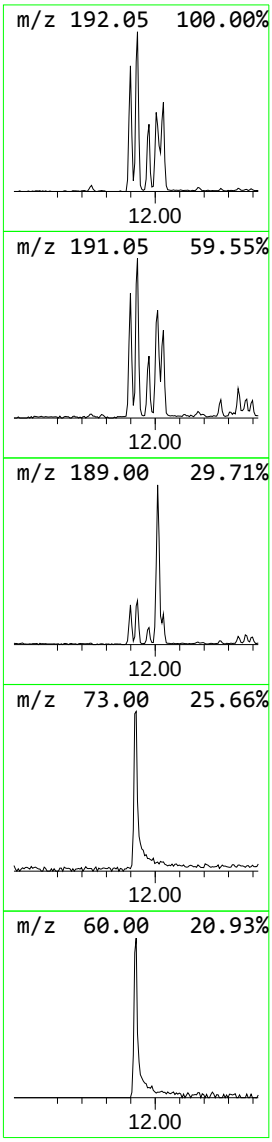
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	4.31 ng	259585	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	98
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	91





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-N-1

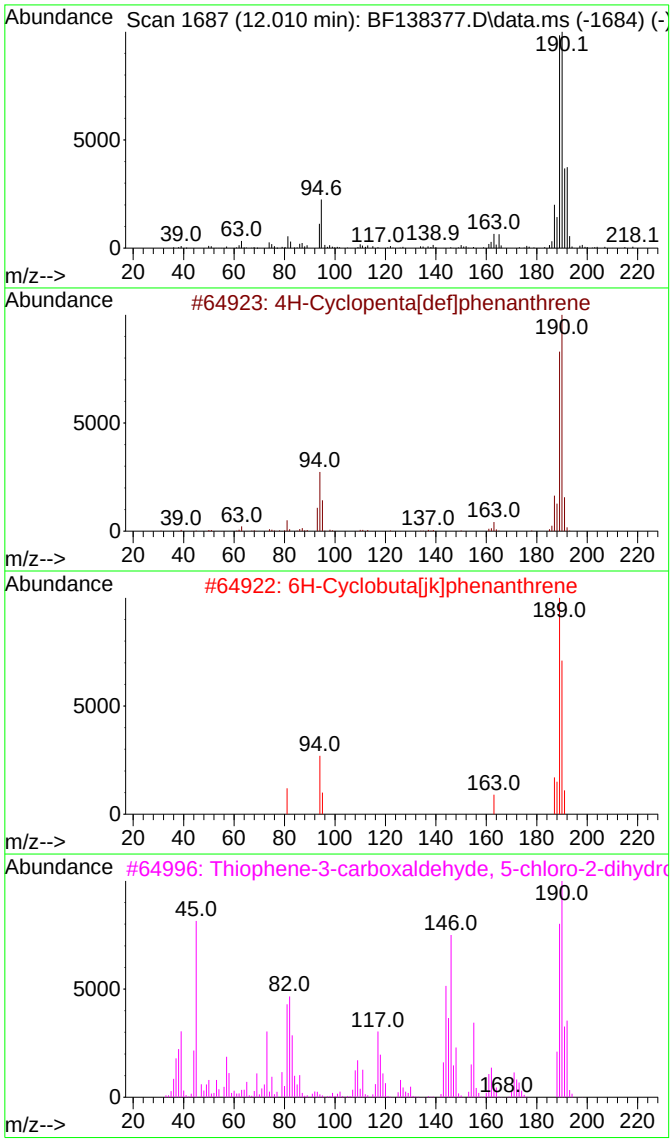
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

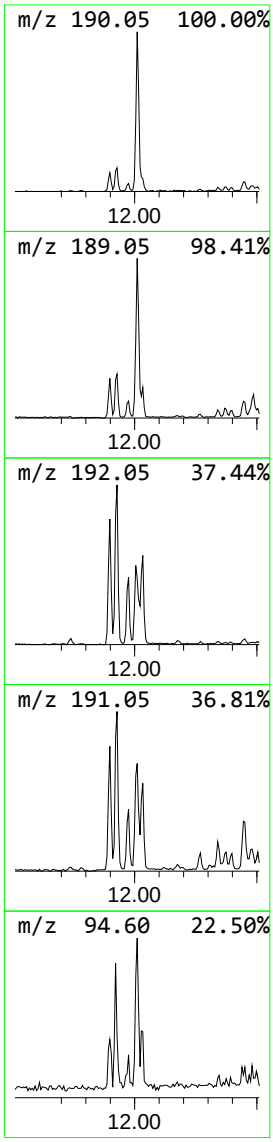
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.010	3.35 ng	201723	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	72
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	53
4	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
5	Methyl diselenide	190	C2H6Se2	007101-31-7	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138377.D
Acq On : 27 Jun 2024 20:39
Operator : CG\JU
Sample : P3077-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-N-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

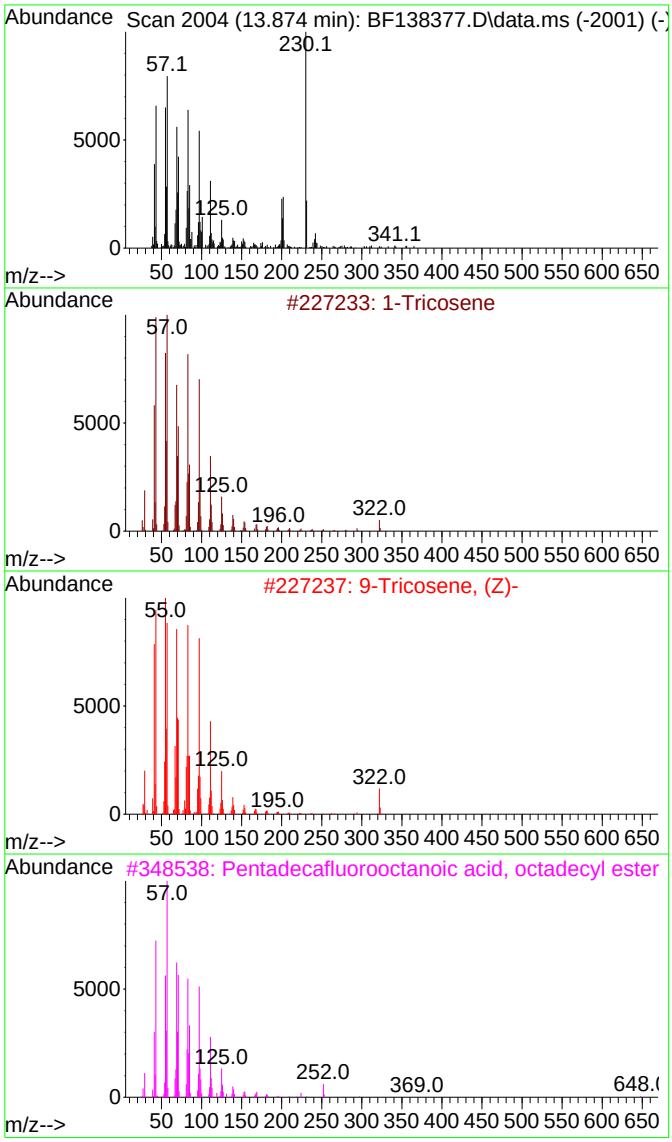
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

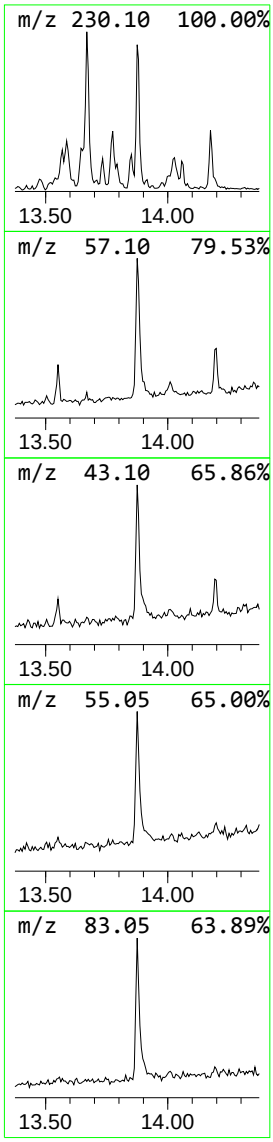
****

Peak Number 7 1-Tricosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.03 ng	282162	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	86
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	81
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	64
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
5	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138377.D
Acq On : 27 Jun 2024 20:39
Operator : CG\JU
Sample : P3077-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-N-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

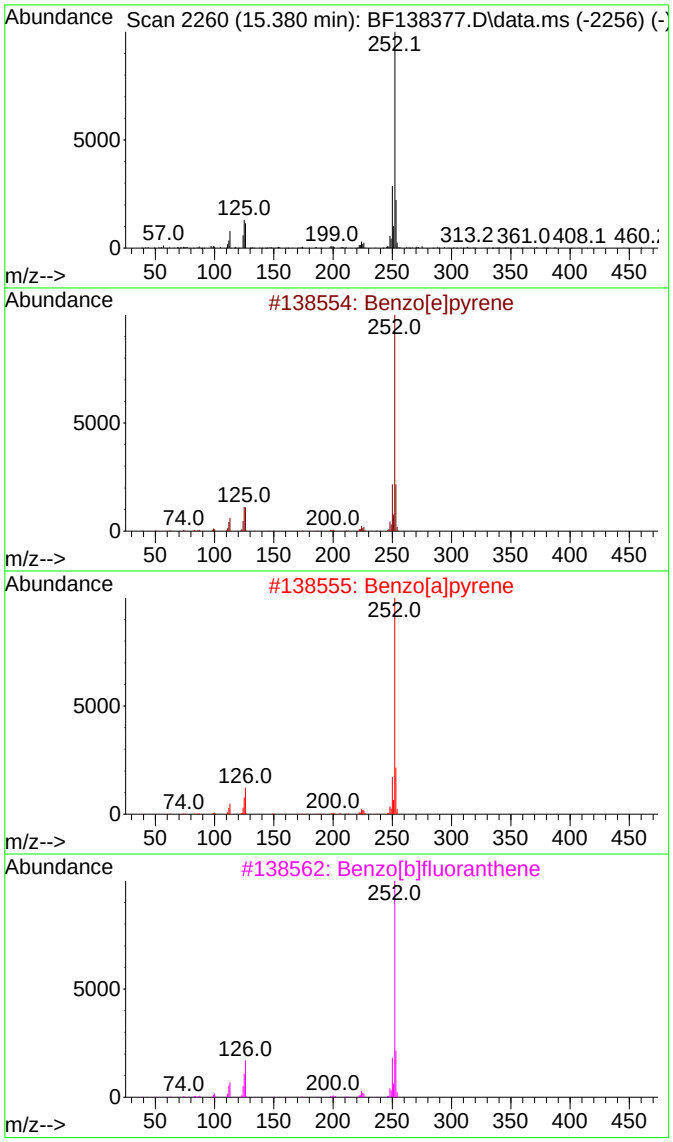
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

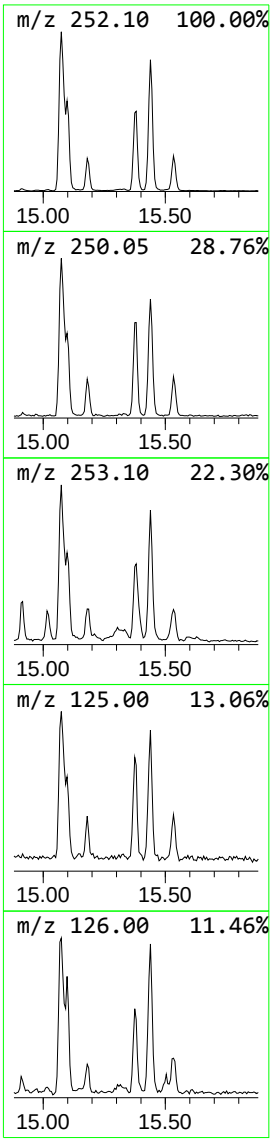
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	4.81 ng	218183	Perylene-d12	15.504

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	97
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
5	Perylene	252	C20H12	000198-55-0	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138377.D
Acq On : 27 Jun 2024 20:39
Operator : CG\JU
Sample : P3077-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-N-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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	39.7	ng	2502120	1	6.881	1259420	20.0
Propylene Glycol	3.399	2.6	ng	162472	1	6.881	1259420	20.0
Propane, 2-meth...	5.099	4.1	ng	257668	1	6.881	1259420	20.0
1-Phenoxypropan...	8.469	2.1	ng	157725	2	8.157	1467010	20.0
Phenanthrene, 2...	11.922	4.3	ng	259585	4	11.398	1205510	20.0
4H-Cyclopenta[d...	12.010	3.4	ng	201723	4	11.398	1205510	20.0
1-Tricosene	13.874	3.0	ng	282162	5	14.033	1861570	20.0
Benzo[e]pyrene	15.380	4.8	ng	218183	6	15.504	906462	20.0