LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138411.D
Acq On : 01 Jul 2024 19:05
Operator : CG\JU
Sample : P3077-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-B-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-BF062824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138411.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	9	16	25	rVB	2227797	2771817	82.87%	9.038%
2	2.287	31	34	41	rVB	33739	46198	1.38%	0.151%
3	3.404	221	224	232	rBV	68465	124065	3.71%	0.405%
4	5.098	508	512	521	rVB	283878	349173	10.44%	1.139%
5	5.504	576	581	584	rBV	3749639	3299615	98.65%	10.759%
6	5.822	631	635	641	rVB	47087	41609	1.24%	0.136%
7	6.510	747	752	755	rBV	3670601	3344612	100.00%	10.906%
8	6.698	781	784	789	rBV	76499	64122	1.92%	0.209%
9	6.875	810	814	817	rBV	1531011	1230056	36.78%	4.011%
10	7.434	904	909	912	rBV	2329914	2146437	64.18%	6.999%
11	7.687	948	952	959	rVB	152689	117099	3.50%	0.382%
12	8.157	1028	1032	1034	rBV	1669801	1511573	45.19%	4.929%
13	8.369	1064	1068	1074	rVB	44188	38322	1.15%	0.125%
14	8.463	1080	1084	1093	rVB	210033	178147	5.33%	0.581%
15	9.228	1210	1214	1217	rBV	3657466	2840332	84.92%	9.262%
16	9.904	1326	1329	1333	rVV	1678058	1396332	41.75%	4.553%
17	9.939	1333	1335	1339	rVB	54396	43880	1.31%	0.143%
18	10.004	1342	1346	1351	rVB2	97342	125005	3.74%	0.408%
19	10.451	1419	1422	1427	rBV	45841	40330	1.21%	0.132%
20	10.692	1459	1463	1466	rBV	1738197	1397127	41.77%	4.556%
21	10.804	1479	1482	1487	rBV4	41205	60378	1.81%	0.197%
22	11.392	1578	1582	1584	rBV	1189735	1063965	31.81%	3.469%
23	11.416	1584	1586	1589	rVV	282855	223471	6.68%	0.729%
24	11.463	1592	1594	1597	rVB	75585	62791	1.88%	0.205%
25	11.622	1614	1621	1625	rBV	26814	36933	1.10%	0.120%
26	11.916	1668	1671	1675	rBV2	158936	156041	4.67%	0.509%
27	12.004	1682	1686	1688	rBV2	56359	55483	1.66%	0.181%
28	12.474	1763	1766	1772	rVB4	32204	42440	1.27%	0.138%
29	12.598	1784	1787	1791	rBV	431070	370734	11.08%	1.209%
30	12.657	1793	1797	1801	rVB3	87885	92857	2.78%	0.303%
31	12.698	1801	1804	1808	rBV2	47057	54311	1.62%	0.177%
32	12.827	1818	1826	1832	rBV	376423	406149	12.14%	1.324%
33	12.974	1847	1851	1854	rBV	2287056	1946404	58.20%	6.347%
34	13.051	1859	1864	1867	rBV3	21704	36056	1.08%	0.118%
35	13.157	1879	1882	1885	rVB	54164	44515	1.33%	0.145%
36	13.257	1896	1899	1902	rBV2	36428	39036	1.17%	0.127%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138411.D
Acq On : 01 Jul 2024 19:05
Operator : CG\JU
Sample : P3077-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-B-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-BF062824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.451	1928	1932	1935	rBV	2394640	1926713	57.61%	6.283%
38	13.868	2000	2003	2012	rVB2	221786	278519	8.33%	0.908%
39	14.027	2024	2030	2032	rBV2	1145341	1191650	35.63%	3.886%
40	14.051	2032	2034	2040	rVB	201167	176903	5.29%	0.577%
41	14.492	2106	2109	2115	rBV4	76225	146565	4.38%	0.478%
42	14.798	2159	2161	2163	rBV	38579	40462	1.21%	0.132%
43	15.062	2203	2206	2209	rBV	112892	156574	4.68%	0.511%
44	15.368	2255	2258	2264	rVB	69780	97472	2.91%	0.318%
45	15.427	2265	2268	2274	rVB	98336	120613	3.61%	0.393%
46	15.492	2275	2279	2283	rBV	617498	734866	21.97%	2.396%

Sum of corrected areas: 30667752

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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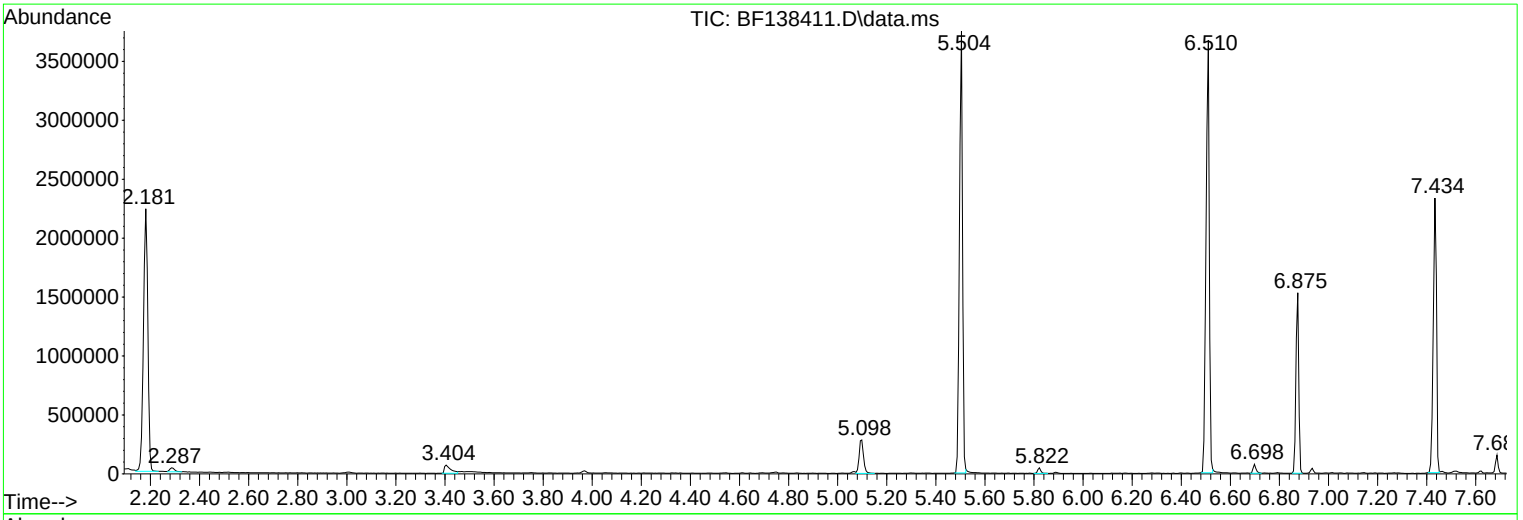
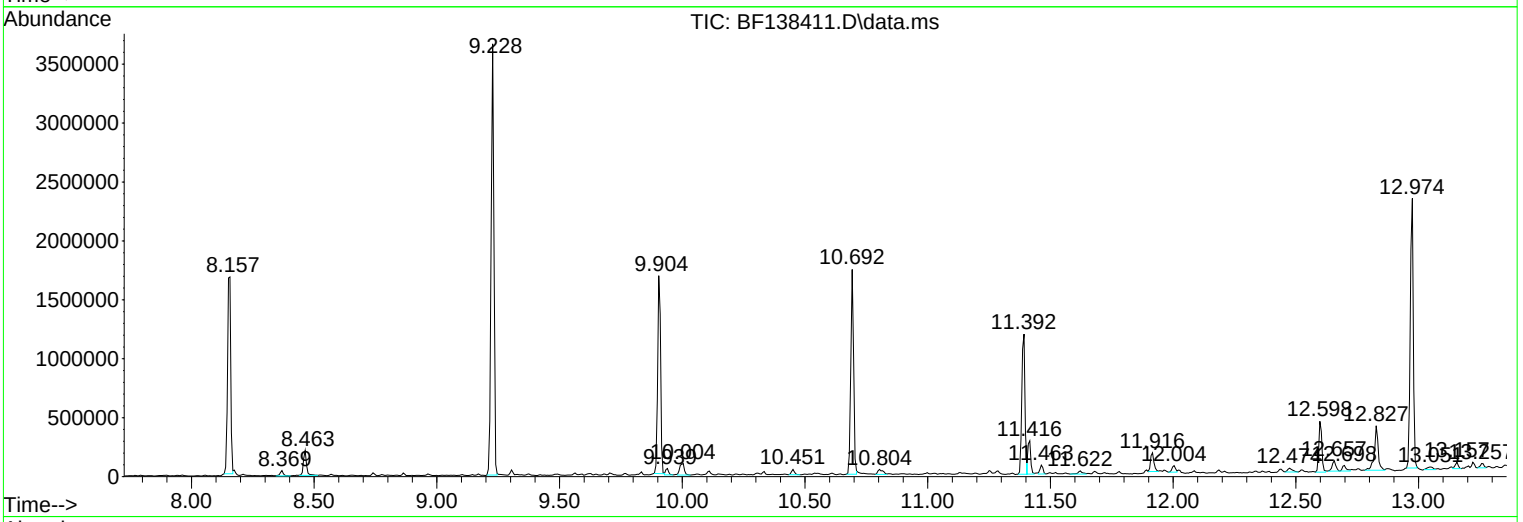
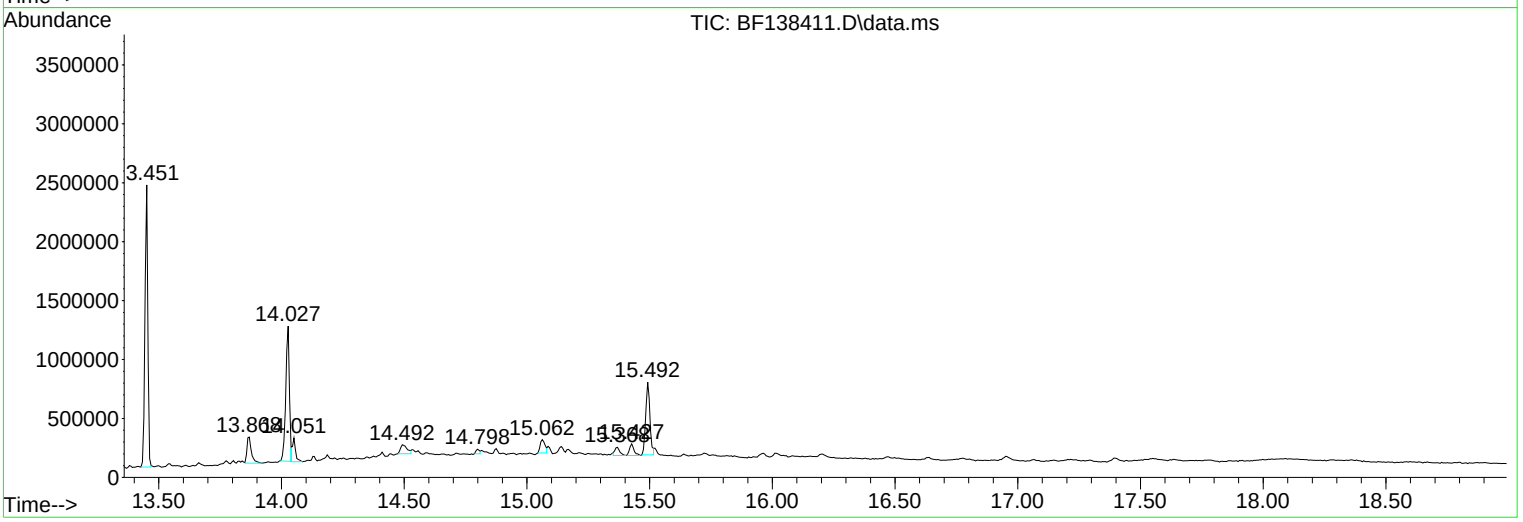
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138411.D
Acq On : 01 Jul 2024 19:05
Operator : CG\JU
Sample : P3077-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

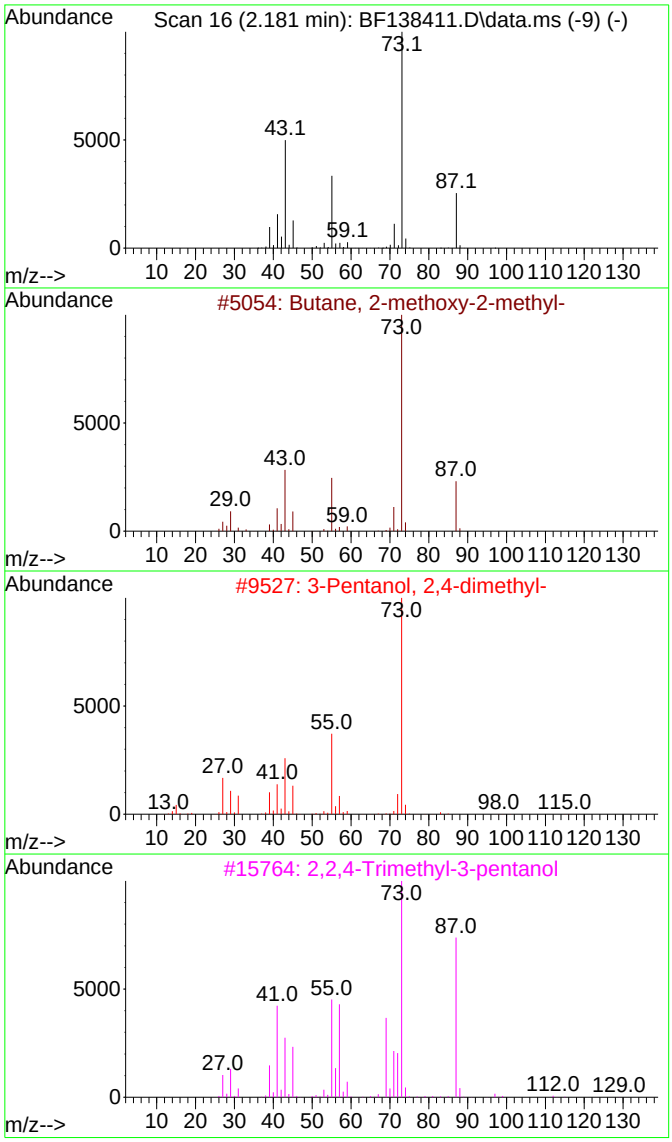
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

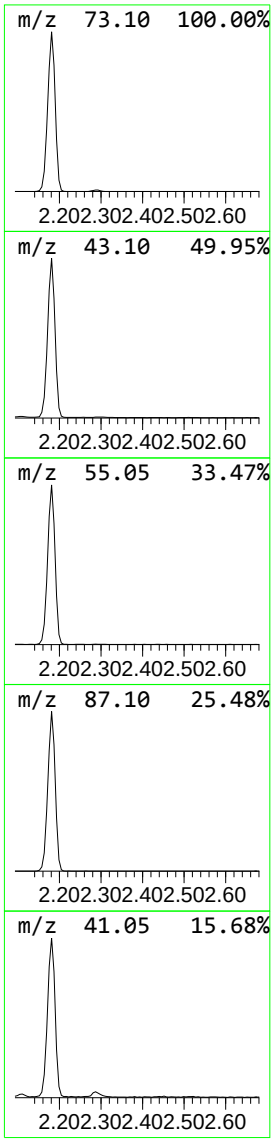
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	45.07 ng	2771820	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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Data File : BF138411.D
Acq On : 01 Jul 2024 19:05
Operator : CG\JU
Sample : P3077-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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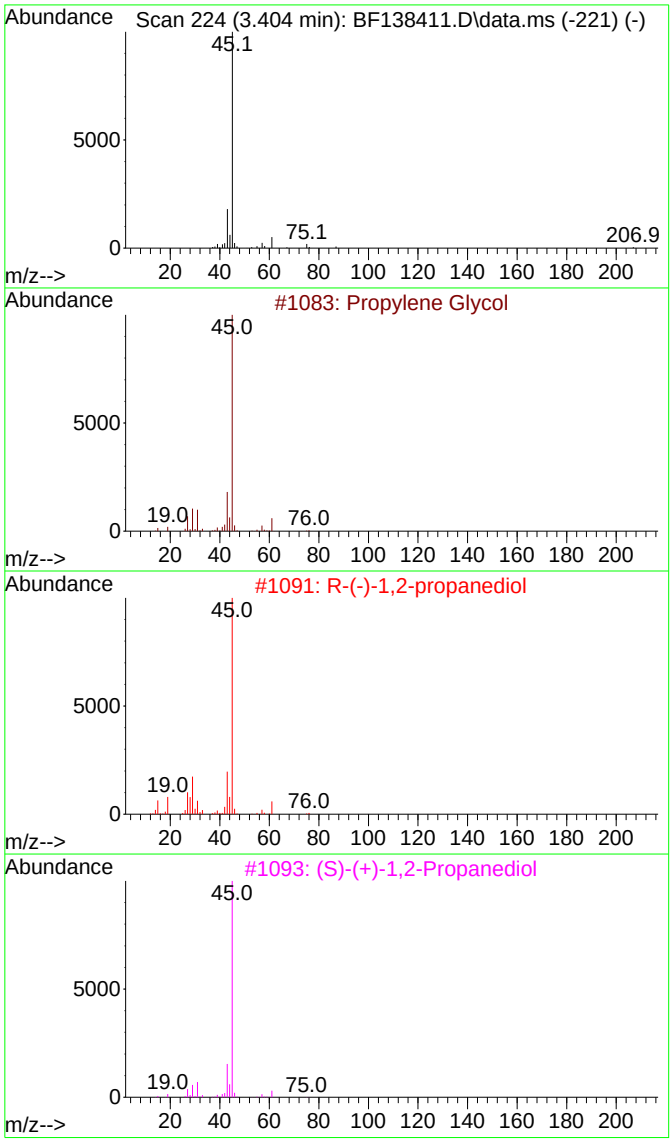
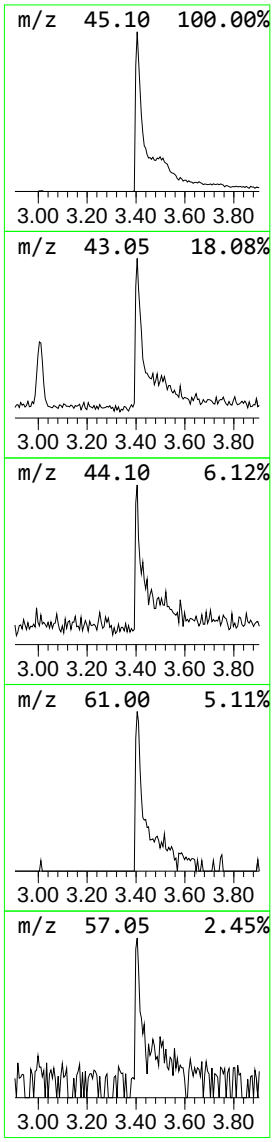
Peak Number 2 Propylene Glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.404	2.02 ng	124065	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
4	Methoxyacetic acid, pentyl ester	160	C8H16O3	168920-35-2	43
5	Ethane, 1,1-diethoxy-	118	C6H14O2	000105-57-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138411.D
Acq On : 01 Jul 2024 19:05
Operator : CG\JU
Sample : P3077-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-B-1

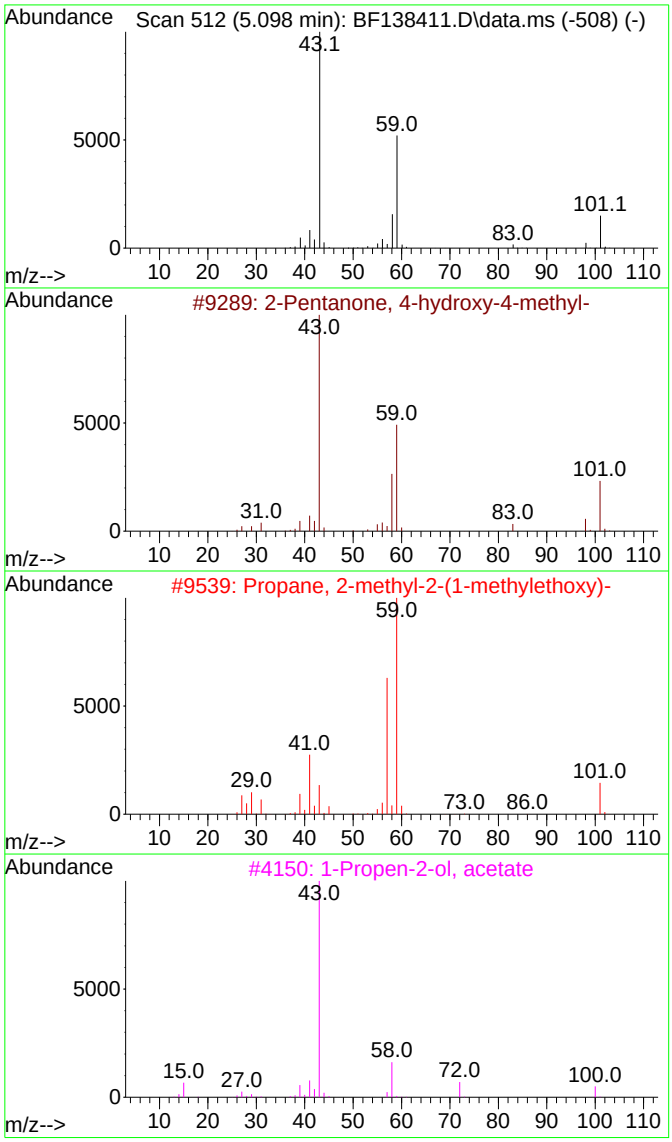
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

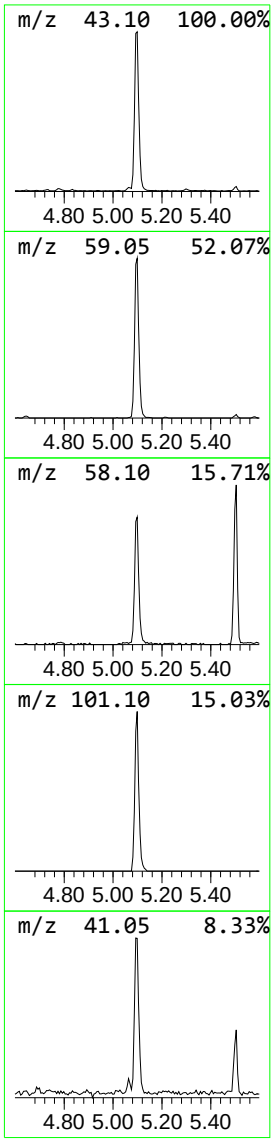
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	5.68 ng	349173	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





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Sample : P3077-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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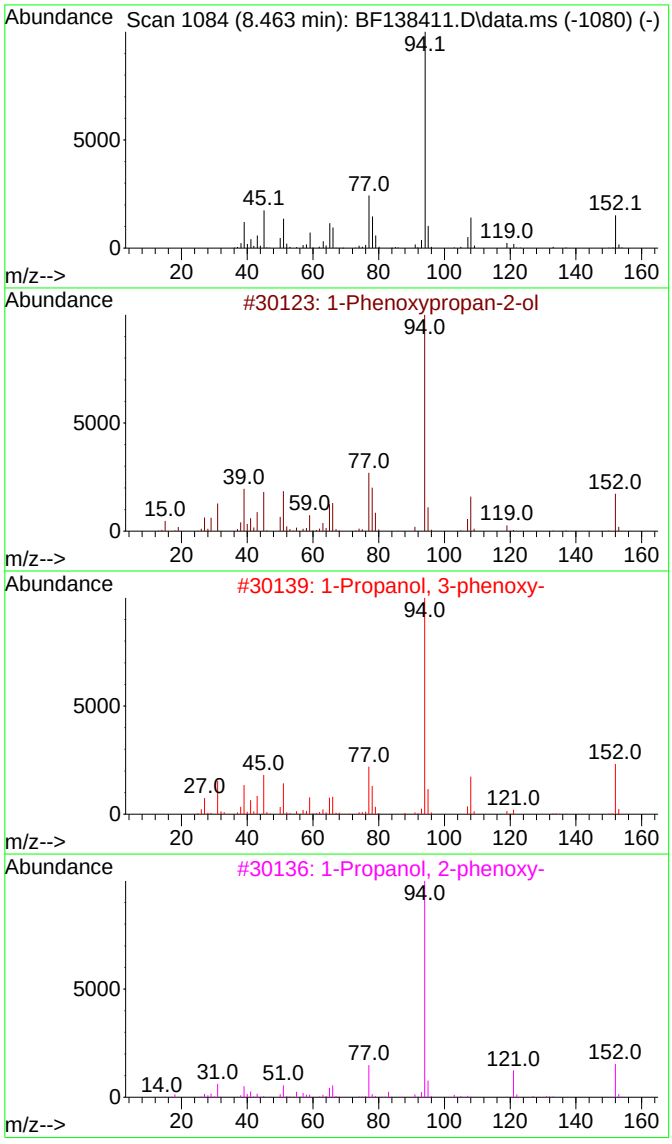
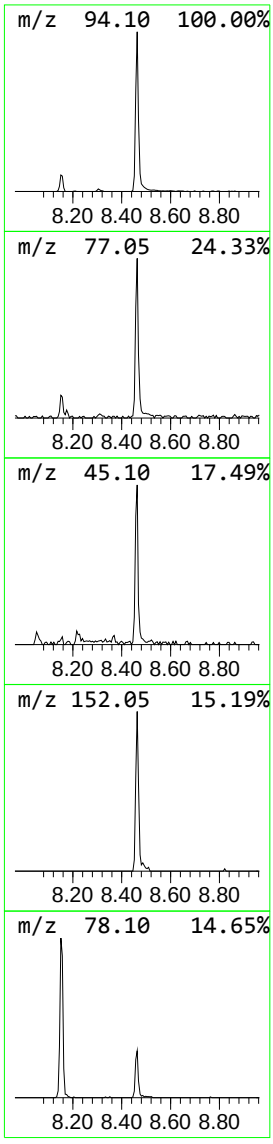
Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.463	2.36 ng	178147	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	91
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





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Data File : BF138411.D
Acq On : 01 Jul 2024 19:05
Operator : CG\JU
Sample : P3077-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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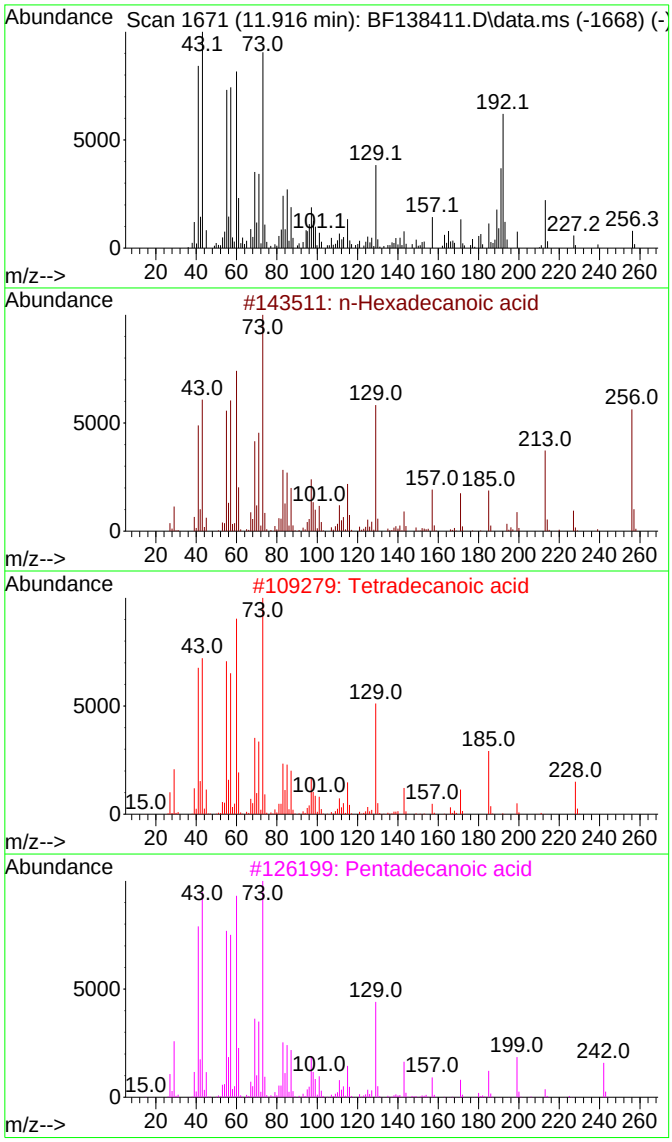
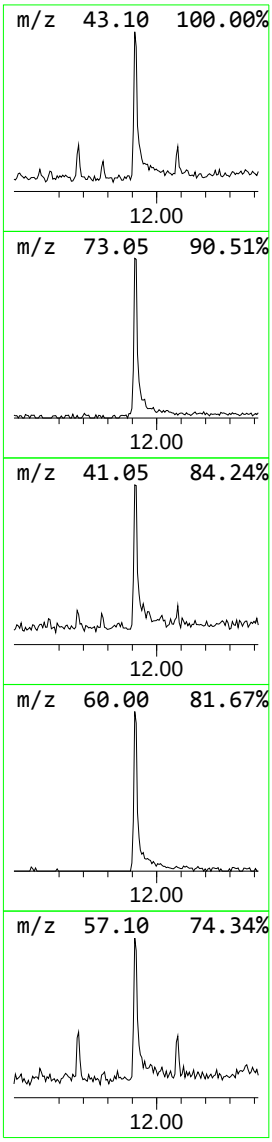
Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.93 ng	156041	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4	Tridecanoic acid	214	C13H26O2	000638-53-9	60
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	59





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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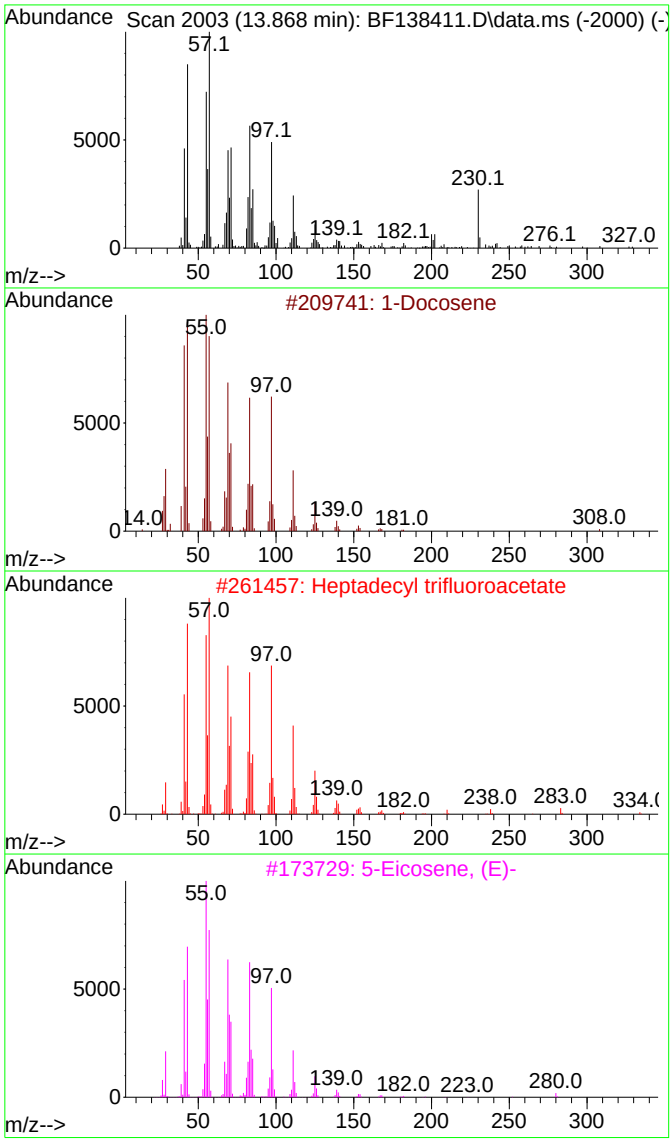
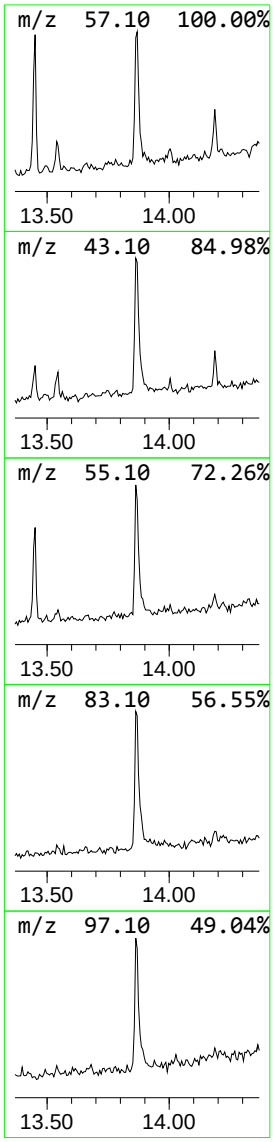
Peak Number 6 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	4.67 ng	278519	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	99
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	90
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90





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Sample : P3077-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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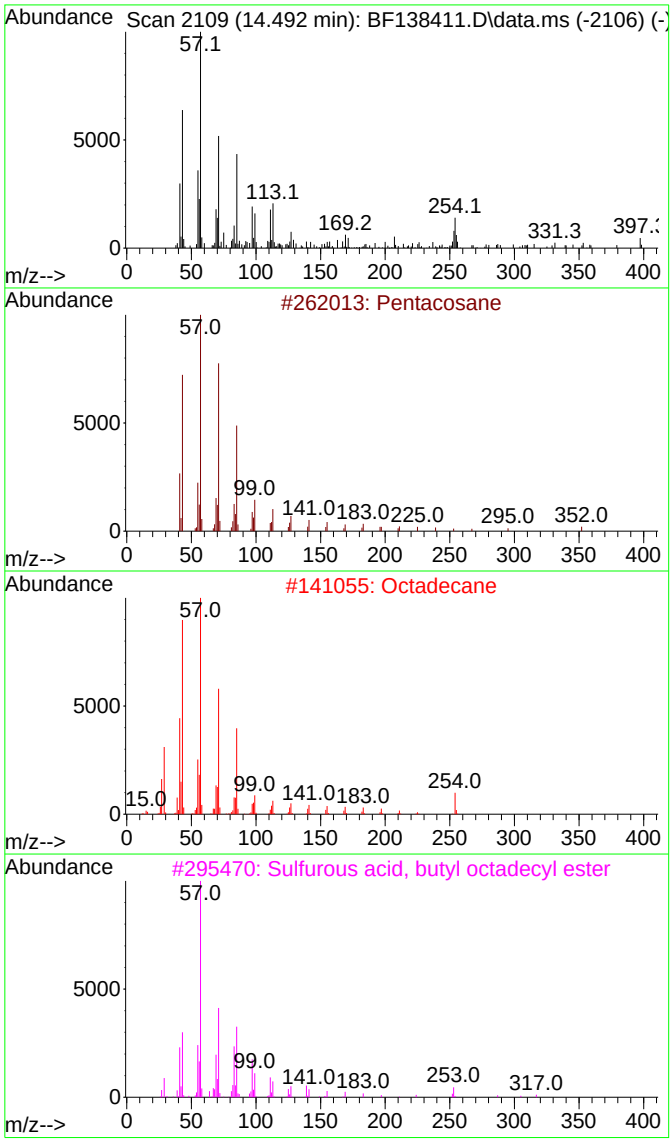
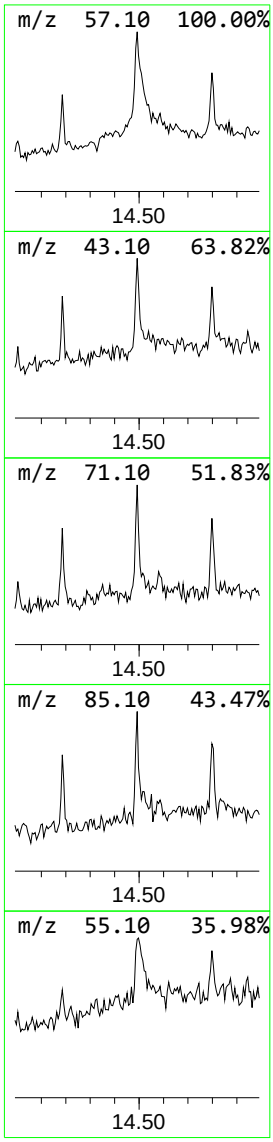
Peak Number 7 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	2.46 ng	146565	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	78
2	Octadecane	254	C18H38	000593-45-3	70
3	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	64
4	Hexadecane	226	C16H34	000544-76-3	64
5	Octacosane	394	C28H58	000630-02-4	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138411.D
Acq On : 01 Jul 2024 19:05
Operator : CG\JU
Sample : P3077-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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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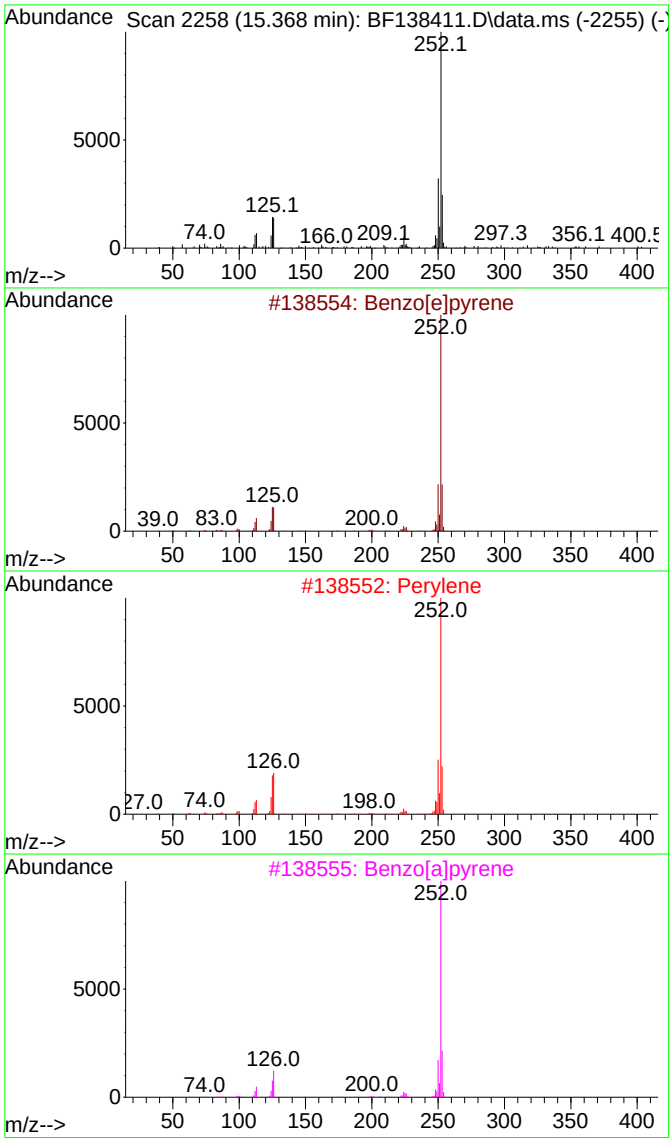
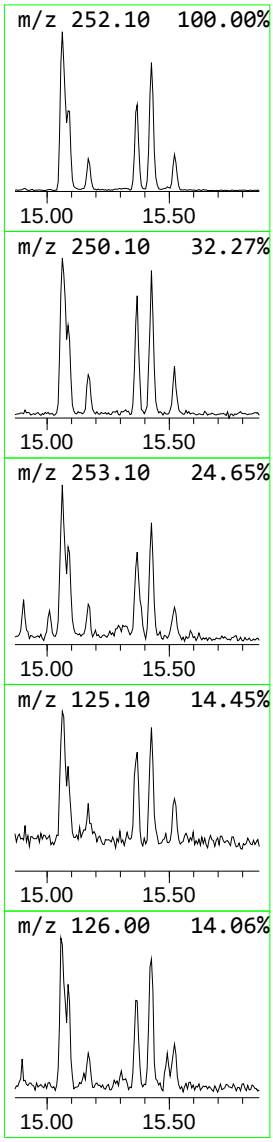
Peak Number 8 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.368	2.65 ng	97472	Perylene-d12	15.492

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Perylene	252	C20H12	000198-55-0	97
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	96





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138411.D
Acq On : 01 Jul 2024 19:05
Operator : CG\JU
Sample : P3077-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-B-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.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...	2.181	45.1	ng	2771820	1	6.875	1230060	20.0
Propylene Glycol	3.404	2.0	ng	124065	1	6.875	1230060	20.0
2-Pentanone, 4-...	5.098	5.7	ng	349173	1	6.875	1230060	20.0
1-Phenoxypropan...	8.463	2.4	ng	178147	2	8.157	1511570	20.0
n-Hexadecanoic ...	11.916	2.9	ng	156041	4	11.392	1063970	20.0
1-Docosene	13.868	4.7	ng	278519	5	14.027	1191650	20.0
Pentacosane	14.492	2.5	ng	146565	5	14.027	1191650	20.0
Benzo[e]pyrene	15.368	2.6	ng	97472	6	15.492	734866	20.0