LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040822\
Data File : BF127726.D
Acq On : 08 Apr 2022 21:21
Operator : CG\JU
Sample : N2329-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-346

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-BF040622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127726.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.334	3	8	14	rVB	299392	386448	7.39%	1.216%
2	2.452	23	28	36	rVB2	38835	56756	1.09%	0.179%
3	2.693	60	69	77	rVB2	34771	81779	1.56%	0.257%
4	3.769	214	252	254	rBV	706018	5227590	100.00%	16.443%
5	5.204	492	496	503	rVB	191089	205190	3.93%	0.645%
6	5.593	556	562	565	rBV	2743553	2910270	55.67%	9.154%
7	6.587	724	731	734	rBV	2776830	3047151	58.29%	9.585%
8	6.963	789	795	798	rBV	1091782	898603	17.19%	2.826%
9	7.528	885	891	894	rBV	2067625	1968177	37.65%	6.191%
10	8.245	1009	1013	1017	rBV	1244657	1104698	21.13%	3.475%
11	9.322	1191	1196	1200	rBV	3079800	2980533	57.02%	9.375%
12	10.010	1307	1313	1316	rVB	1507435	1287852	24.64%	4.051%
13	10.798	1443	1447	1450	rBV	2597686	2268323	43.39%	7.135%
14	11.039	1485	1488	1491	rBV	141420	102246	1.96%	0.322%
15	11.304	1529	1533	1537	rBV	86085	99178	1.90%	0.312%
16	11.498	1563	1566	1569	rBV	1321933	1251995	23.95%	3.938%
17	11.522	1569	1570	1574	rVB	175088	118828	2.27%	0.374%
18	12.016	1648	1654	1660	rBV2	171511	295442	5.65%	0.929%
19	12.110	1668	1670	1673	rBV2	79188	81157	1.55%	0.255%
20	12.474	1729	1732	1736	rBV	185512	200515	3.84%	0.631%
21	12.551	1742	1745	1748	rVB	80860	77923	1.49%	0.245%
22	12.639	1757	1760	1766	rBV3	42511	56317	1.08%	0.177%
23	12.716	1770	1773	1777	rVB	286543	235997	4.51%	0.742%
24	12.945	1807	1812	1819	rBV	277130	338463	6.47%	1.065%
25	13.092	1832	1837	1840	rBV	2660460	2358347	45.11%	7.418%
26	13.163	1845	1849	1856	rVB5	43842	75045	1.44%	0.236%
27	13.380	1882	1886	1889	rVB2	67032	62355	1.19%	0.196%
28	13.510	1904	1908	1919	rBV2	247869	317828	6.08%	1.000%
29	13.980	1985	1988	2001	rVB2	321376	353971	6.77%	1.113%
30	14.151	2009	2017	2019	rBV2	882592	967004	18.50%	3.042%
31	14.174	2019	2021	2027	rVB	137653	124308	2.38%	0.391%
32	14.245	2028	2033	2039	rBV3	74139	127577	2.44%	0.401%
33	14.427	2058	2064	2074	rBV	202303	274588	5.25%	0.864%
34	14.533	2078	2082	2086	rVV	54313	71853	1.37%	0.226%
35	14.621	2092	2097	2101	rBV4	40956	78450	1.50%	0.247%
36	15.015	2161	2164	2169	rBV2	46210	54319	1.04%	0.171%

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Misc :
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Instrument :
BNA_F
ClientSampleId :
RBR-346

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-BF040622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.221	2194	2199	2207	rBV	103562	241855	4.63%	0.761%
38	15.374	2222	2225	2234	rBV2	62978	104175	1.99%	0.328%
39	15.539	2249	2253	2260	rVB	70875	98527	1.88%	0.310%
40	15.604	2260	2264	2269	rBV	91286	123149	2.36%	0.387%
41	15.680	2271	2277	2281	rBV	608798	837722	16.03%	2.635%
42	16.233	2367	2371	2375	rBV5	35579	56744	1.09%	0.178%
43	17.227	2534	2540	2551	rVB3	40735	100140	1.92%	0.315%
44	17.709	2613	2622	2627	rBV2	33978	83094	1.59%	0.261%

Sum of corrected areas: 31792482

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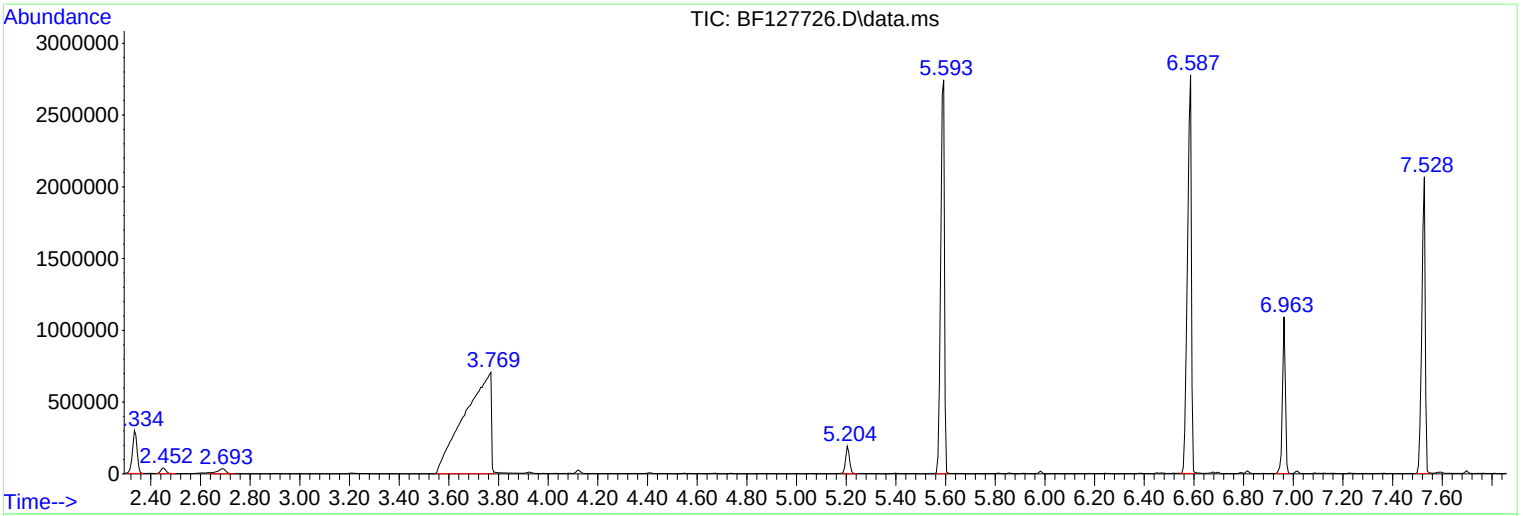
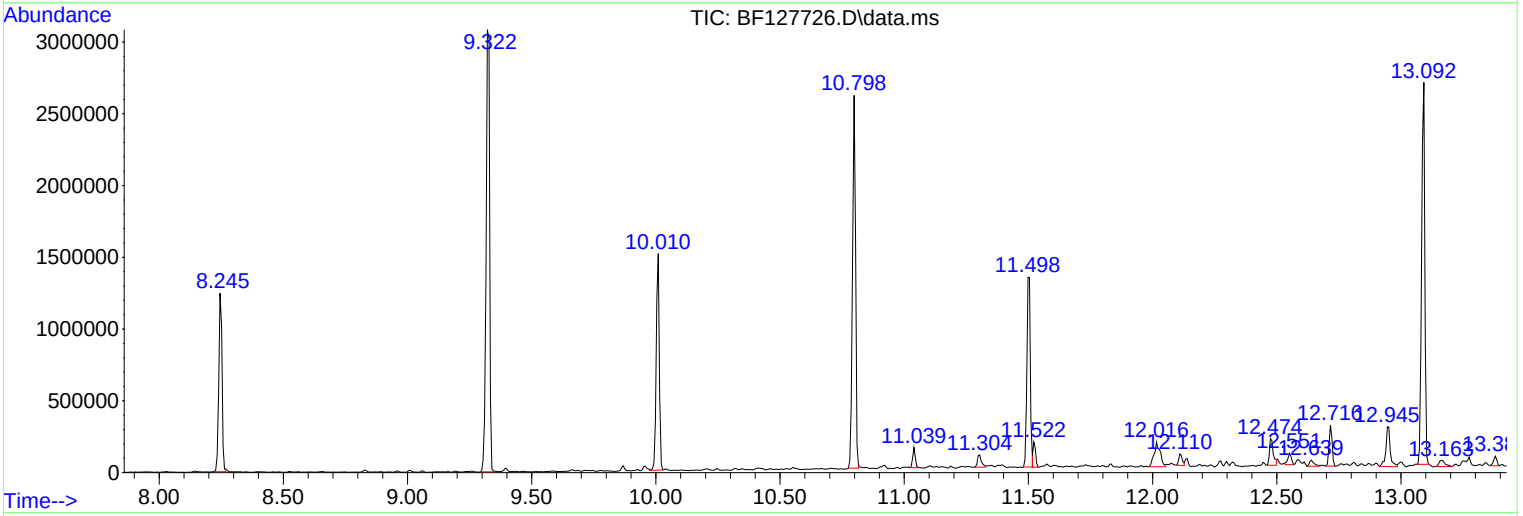
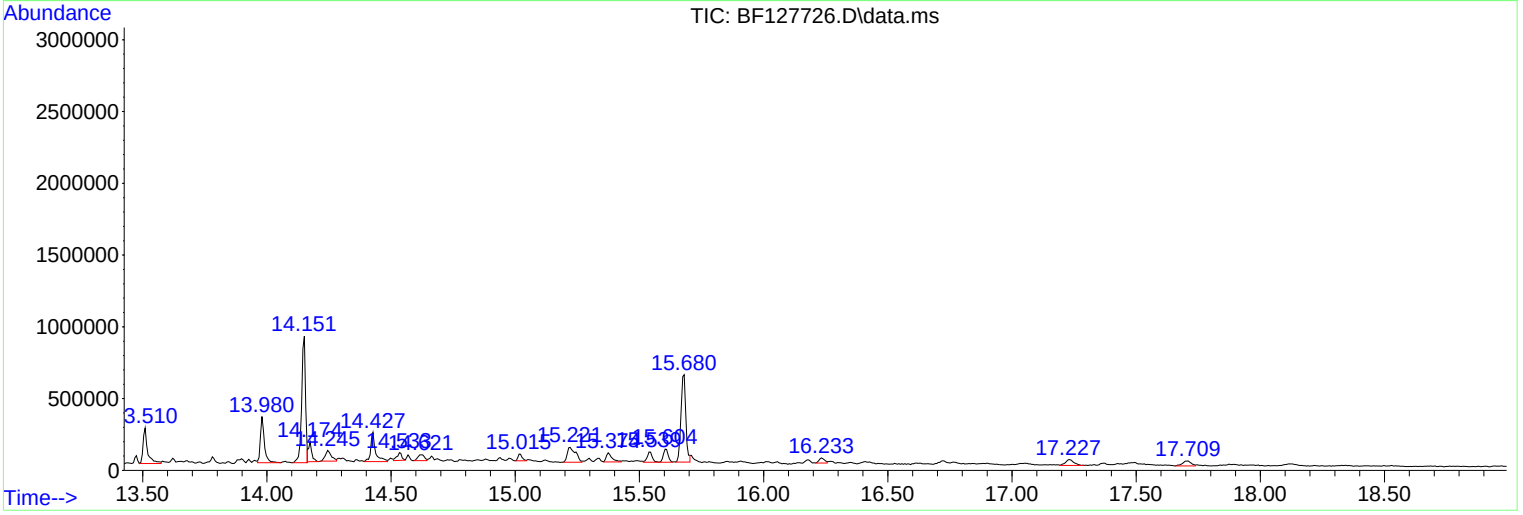
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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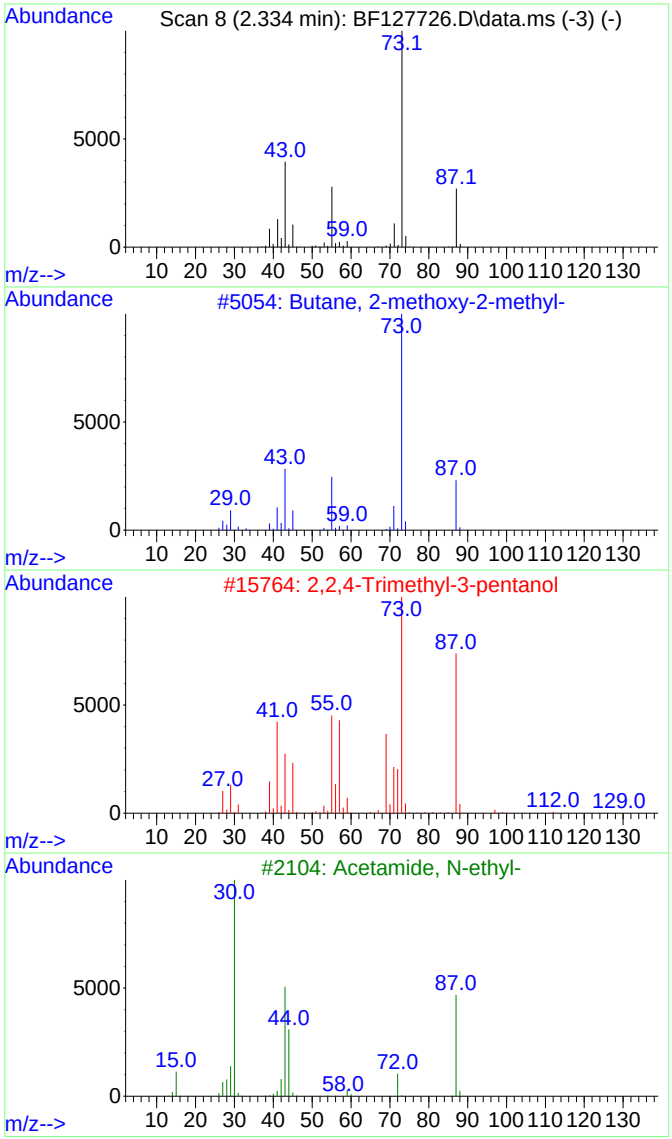
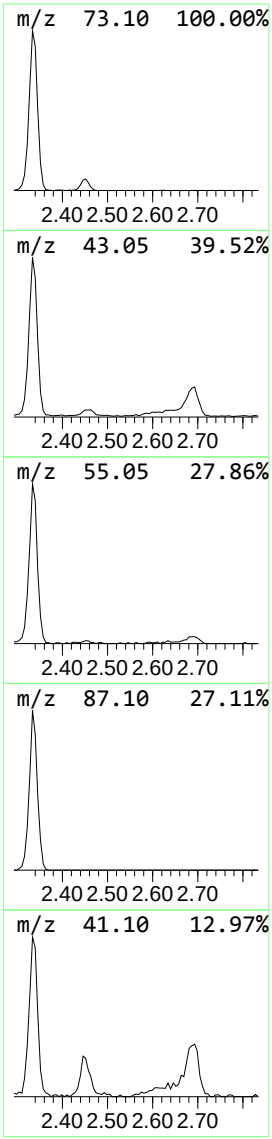
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.334	8.60 ng	386448	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Operator : CG\JU
Sample : N2329-03
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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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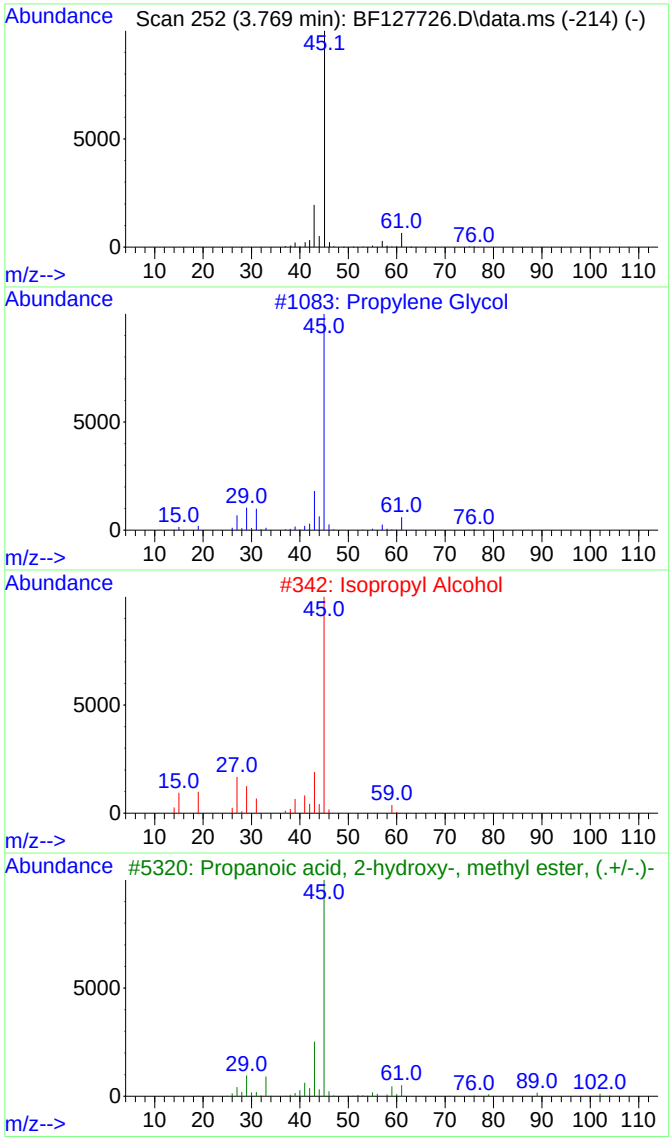
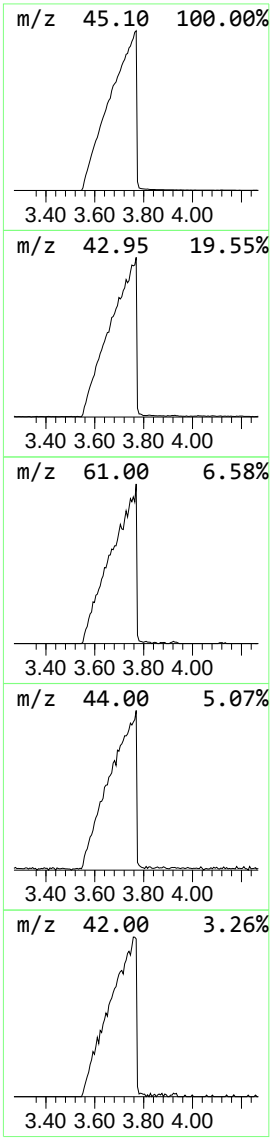
Peak Number 2 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.769	116.35 ng	5227590	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9





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Acq On : 08 Apr 2022 21:21
Operator : CG\JU
Sample : N2329-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

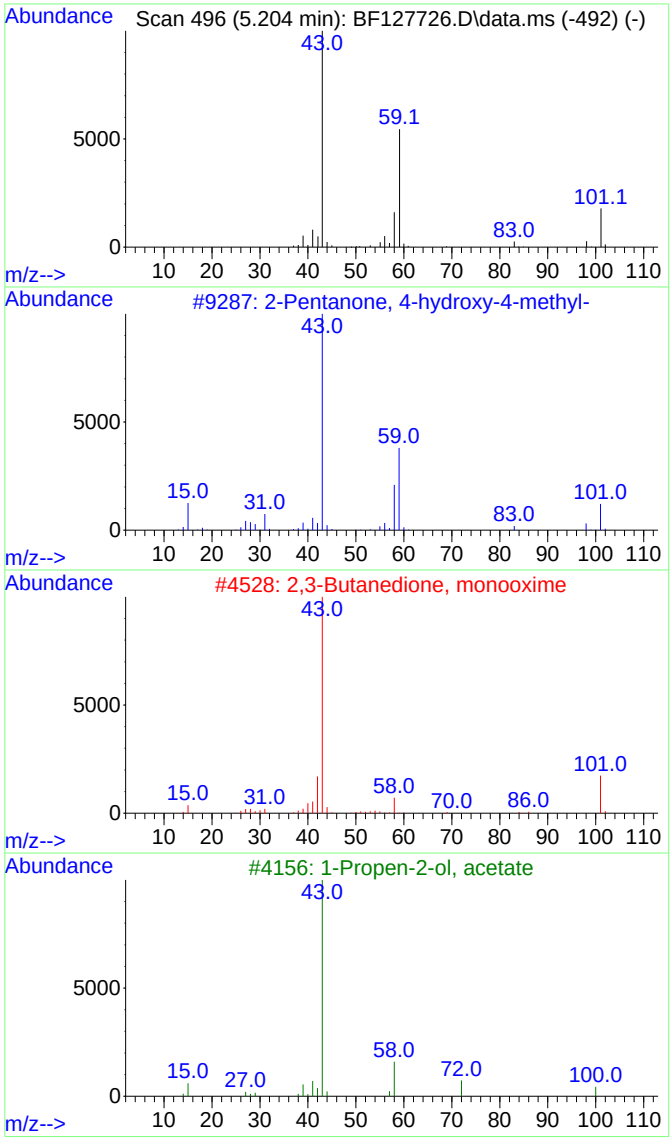
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

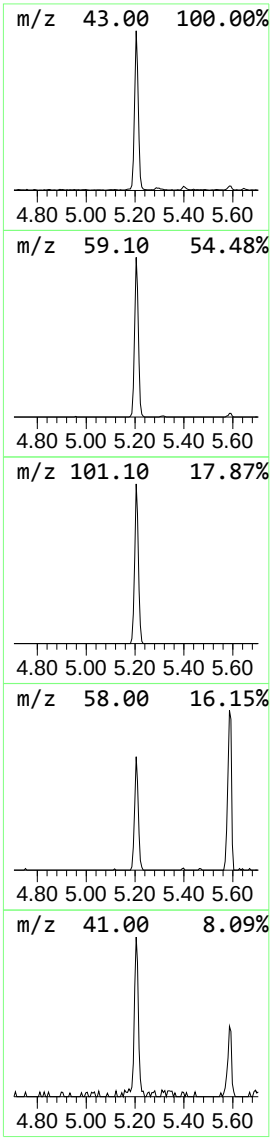
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.204	4.57 ng	205190	1,4-Dichlorobenzene-d4	6.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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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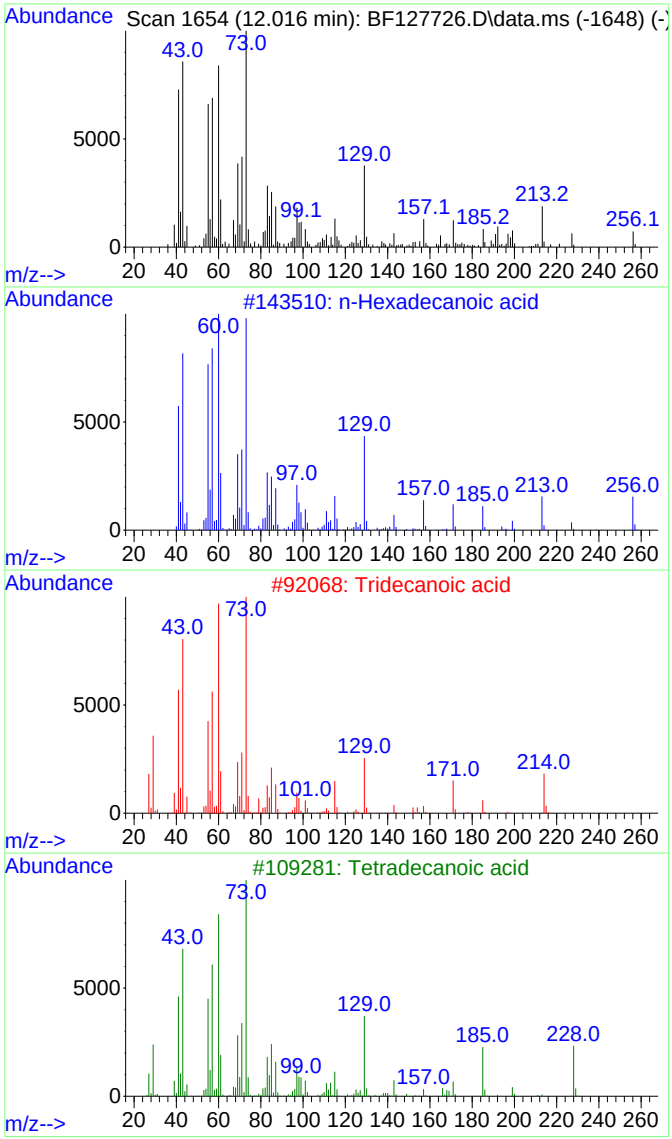
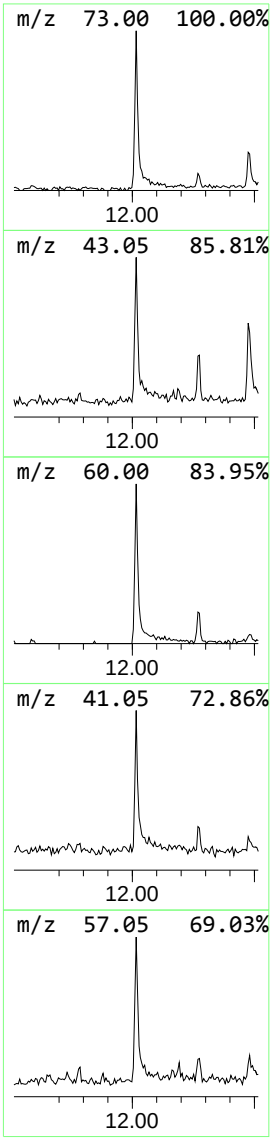
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.016	4.72 ng	295442	Phenanthrene-d10	11.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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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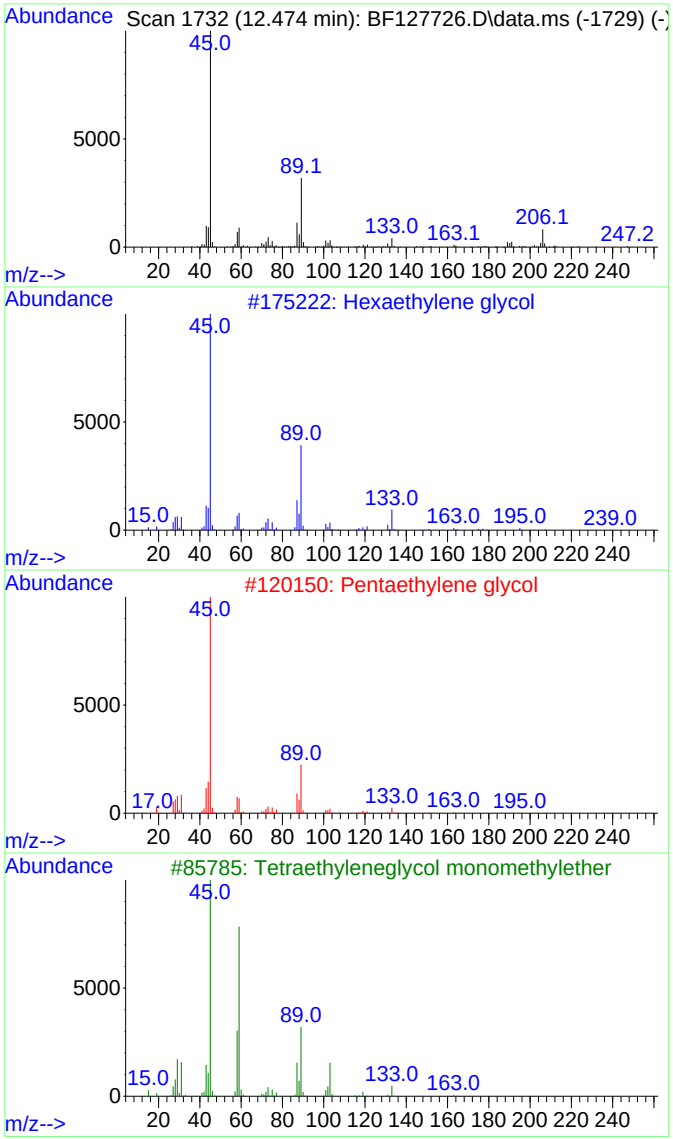
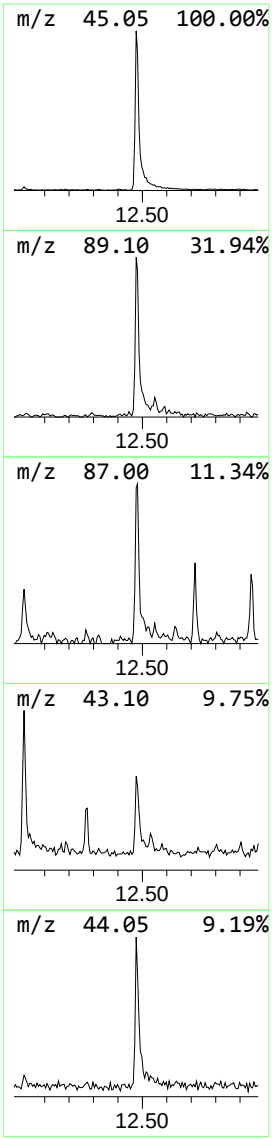
Peak Number 5 Hexaethylene glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.474	3.20 ng	200515	Phenanthrene-d10	11.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	87
2	Pentaethylene glycol	238	C10H22O6	004792-15-8	86
3	Tetraethyleneglycol monomethylether	208	C9H20O5	023783-42-8	78
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	72
5	Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	64





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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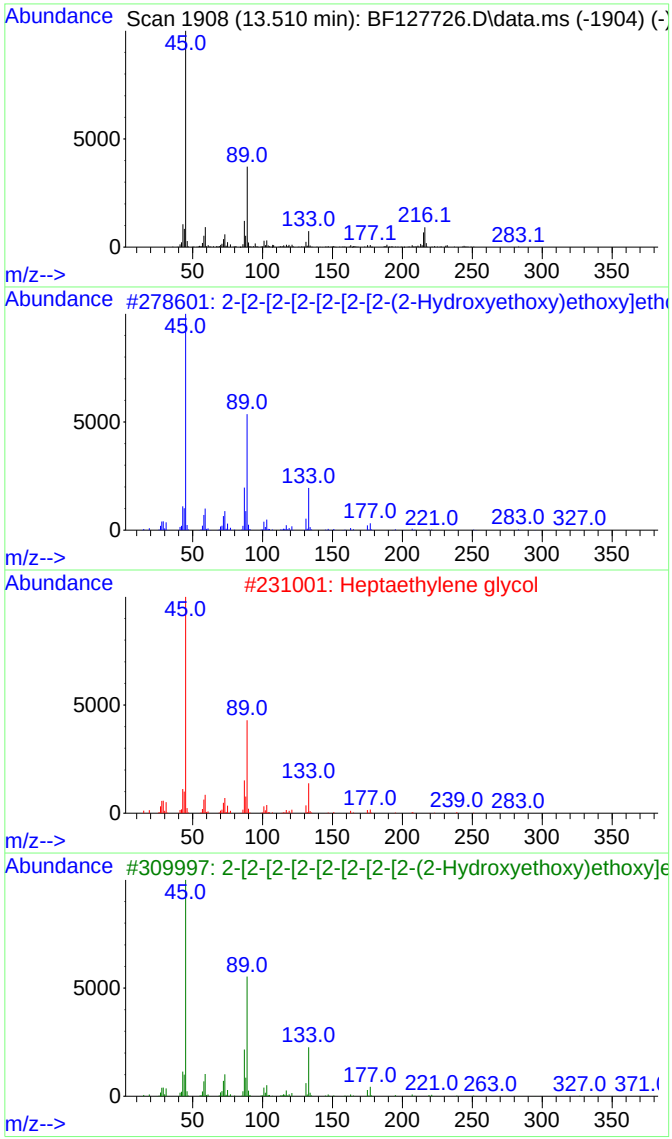
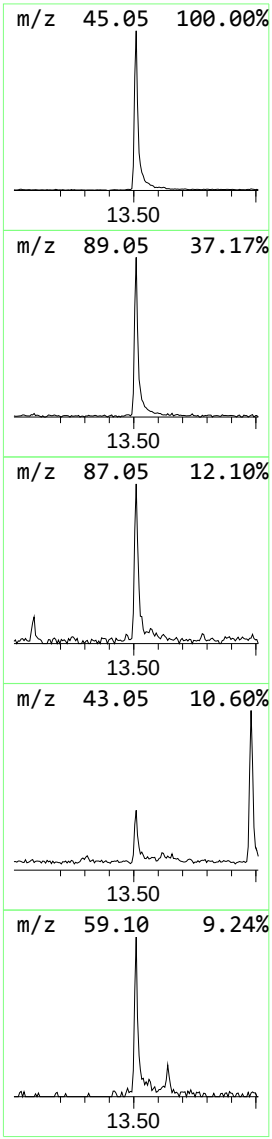
Peak Number 6 2-[2-[2-[2-[2-[2-[2-(2-Hydr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.510	6.57 ng	317828	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	58
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	58
3	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	58
4	Hexaethylene glycol	282	C12H26O7	002615-15-8	58
5	Acetaldehyde, tetramer	176	C8H16O4	000108-62-3	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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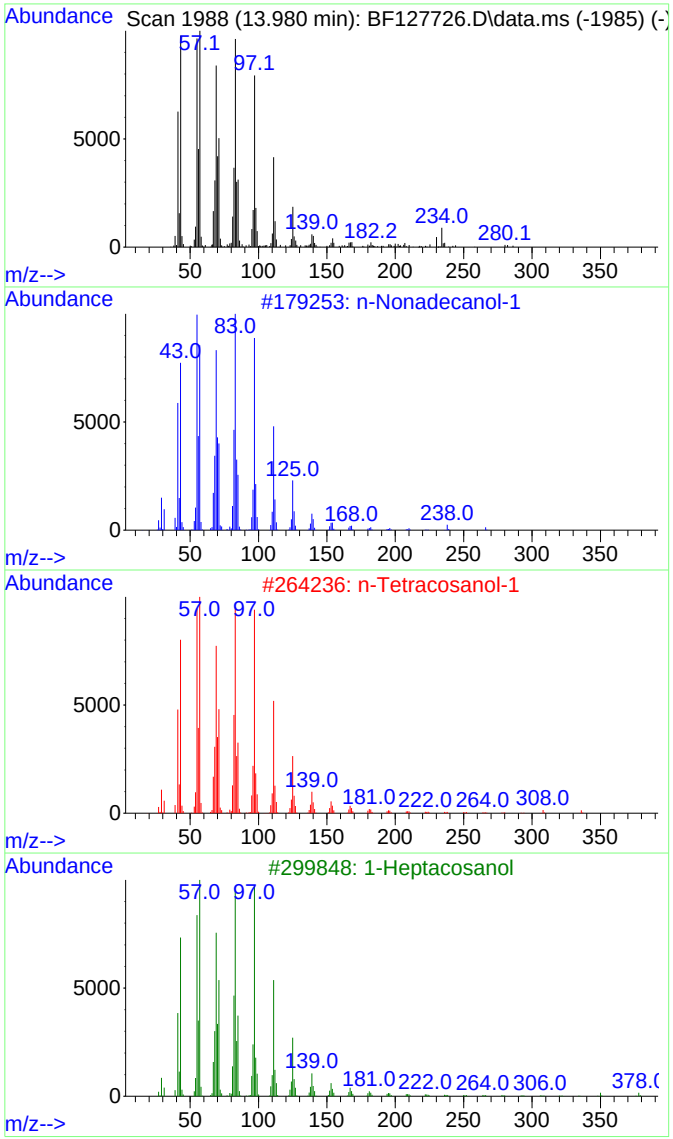
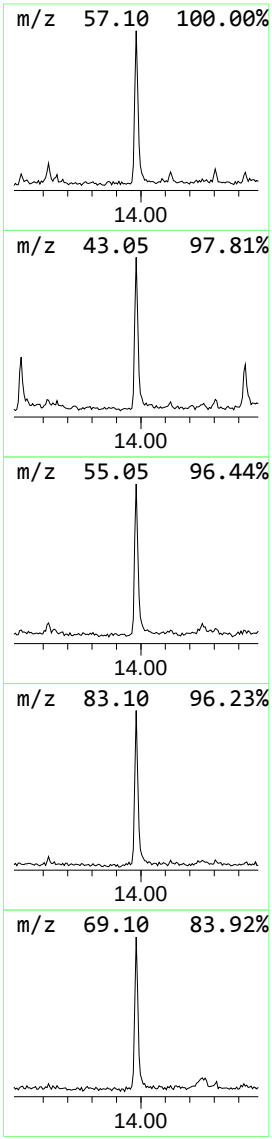
Peak Number 7 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	7.32 ng	353971	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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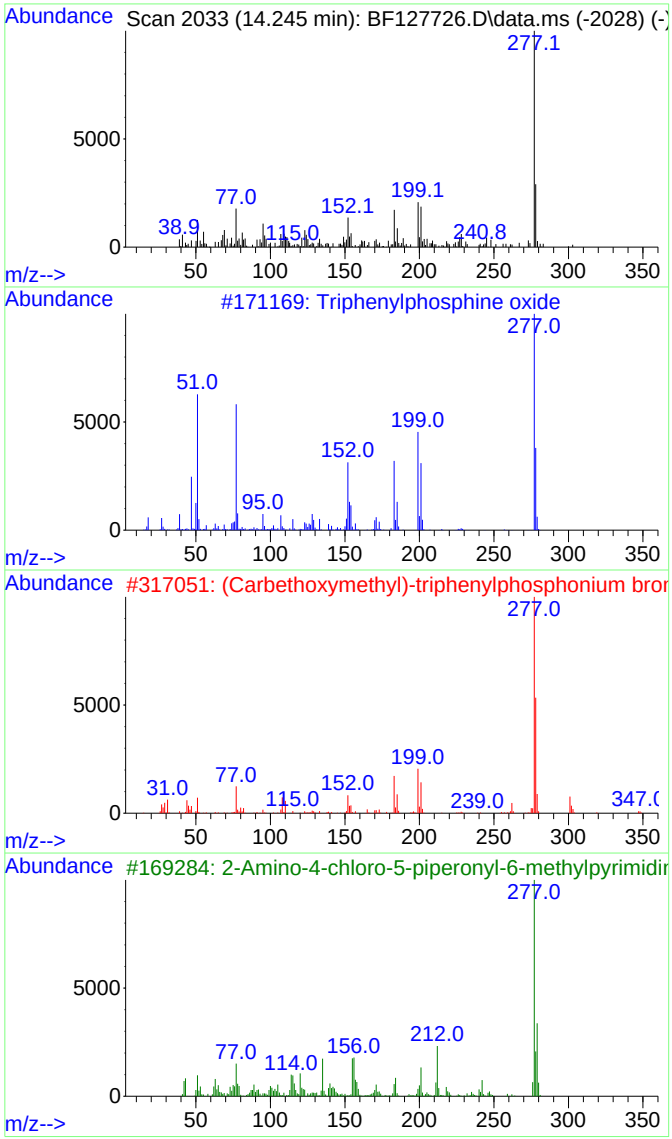
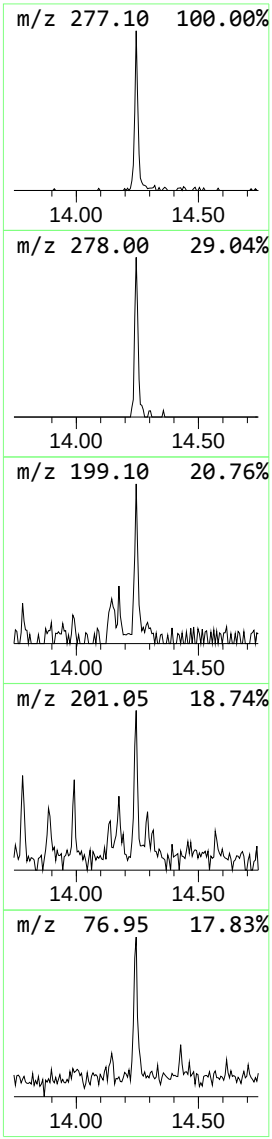
Peak Number 8 Triphenylphosphine oxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.245	2.64 ng	127577	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	59
3	2-Amino-4-chloro-5-piperonyl-6-m...	277	C13H12ClN3O2	1010257-38-4	50
4	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	49
5	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	47





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Data File : BF127726.D
Acq On : 08 Apr 2022 21:21
Operator : CG\JU
Sample : N2329-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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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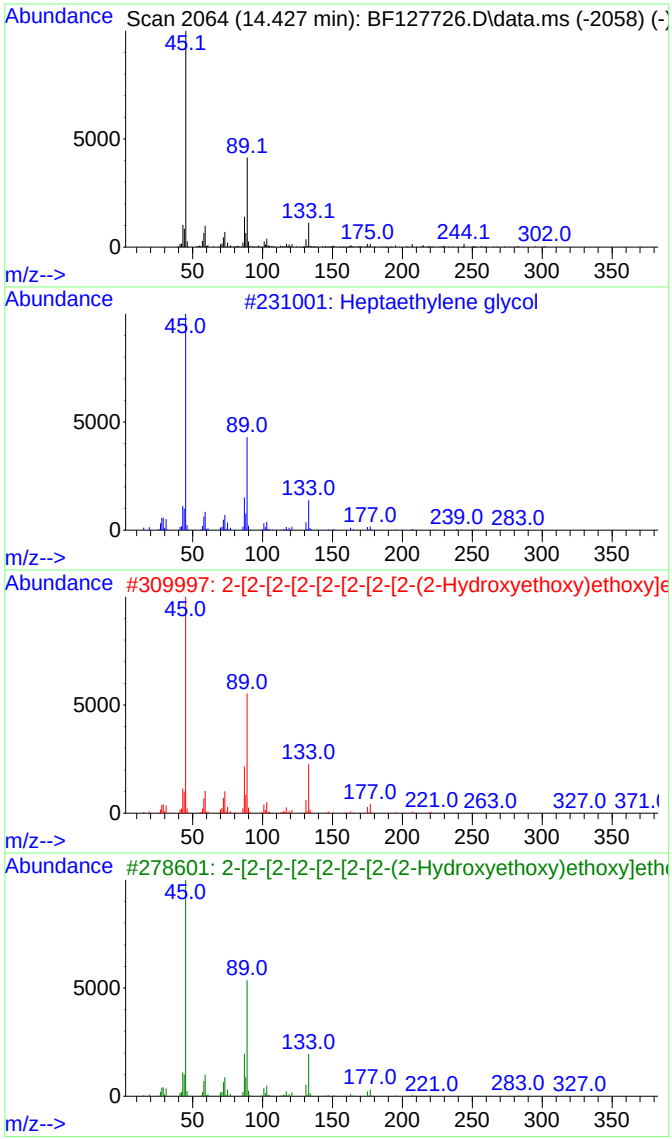
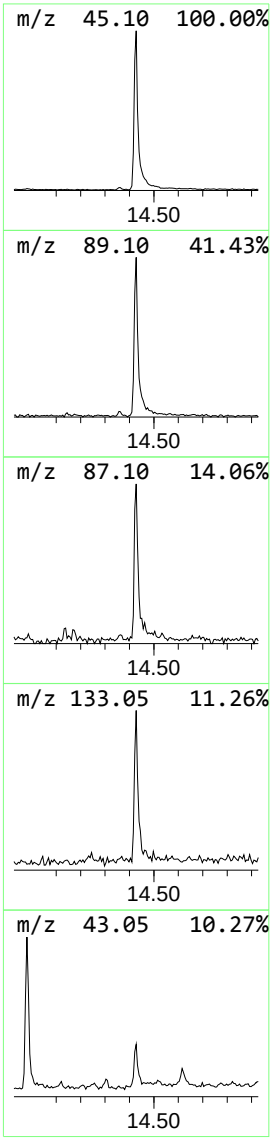
Peak Number 9 Heptaethylene glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.427	5.68 ng	274588	Chrysene-d12	14.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	91
2	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	91
3	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
4	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	005579-66-8	83
5	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	006809-70-7	80





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Data File : BF127726.D
Acq On : 08 Apr 2022 21:21
Operator : CG\JU
Sample : N2329-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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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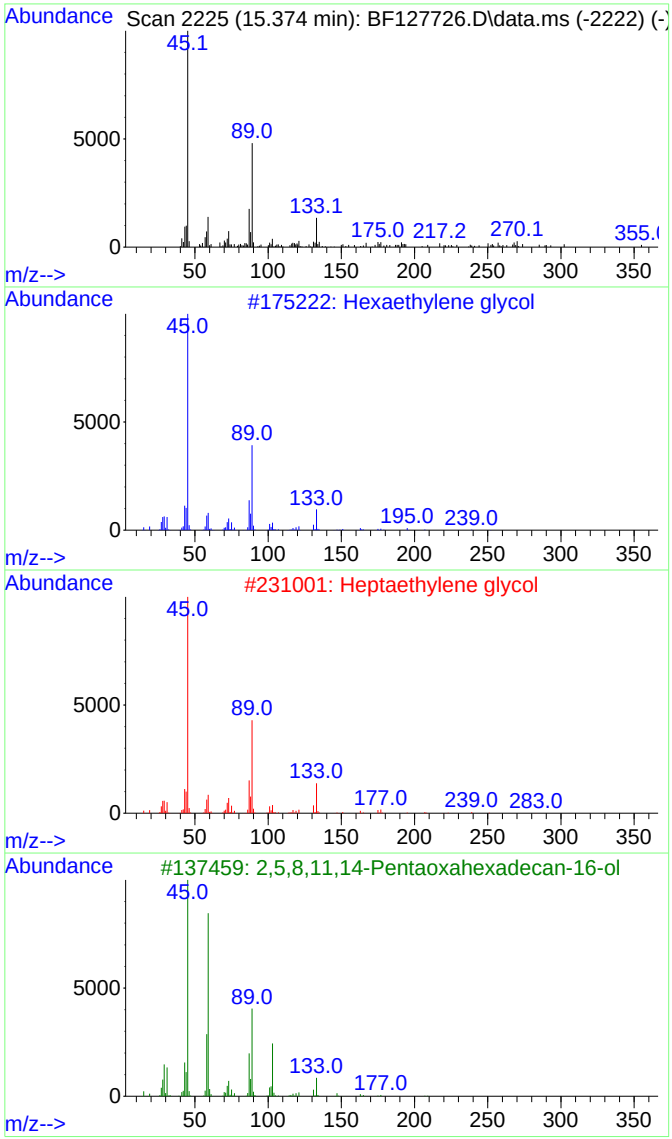
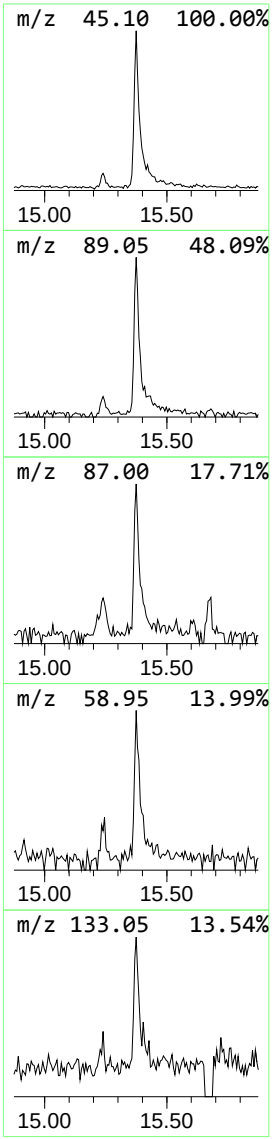
Peak Number 10 2,5,8,11,14-Pentaoxahexadec... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	2.49 ng	104175	Perylene-d12	15.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	90
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	87
3	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	80
4	15-Crown-5	220	C10H20O5	033100-27-5	78
5	Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	64





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Data File : BF127726.D
Acq On : 08 Apr 2022 21:21
Operator : CG\JU
Sample : N2329-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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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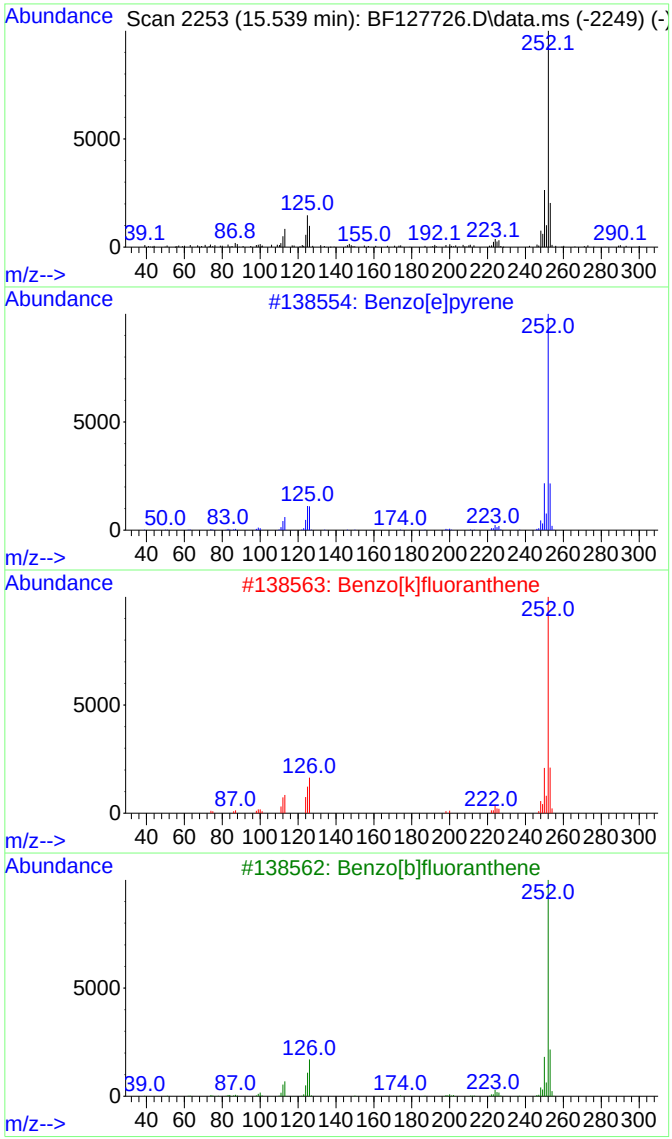
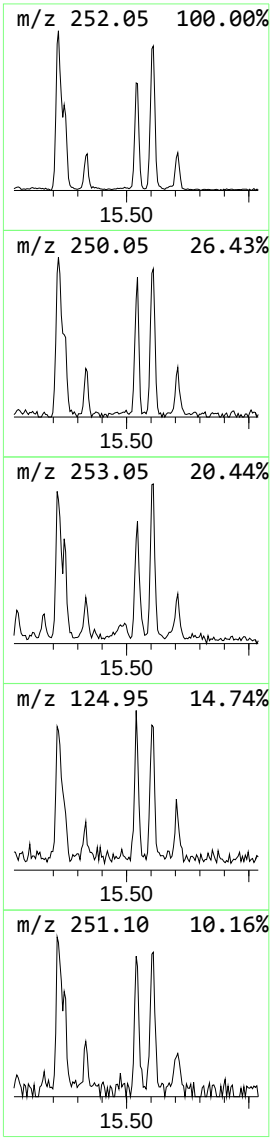
Peak Number 11 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.539	2.35 ng	98527	Perylene-d12	15.680

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	89
4	Perylene	252	C20H12	000198-55-0	81
5	Benzo[a]pyrene	252	C20H12	000050-32-8	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040822\
Data File : BF127726.D
Acq On : 08 Apr 2022 21:21
Operator : CG\JU
Sample : N2329-03
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-346

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF040622.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...	2.334	8.6	ng	386448	1	6.963	898603	20.0
Propylene Glycol	3.769	116.3	ng	5227590	1	6.963	898603	20.0
2-Pentanone, 4-...	5.204	4.6	ng	205190	1	6.963	898603	20.0
n-Hexadecanoic ...	12.016	4.7	ng	295442	4	11.504	1252000	20.0
Hexaethylene gl...	12.474	3.2	ng	200515	4	11.504	1252000	20.0
2-[2-[2-[2-[2-[...	13.510	6.6	ng	317828	5	14.151	967004	20.0
n-Nonadecanol-1	13.980	7.3	ng	353971	5	14.151	967004	20.0
Triphenylphosph...	14.245	2.6	ng	127577	5	14.151	967004	20.0
Heptaethylene g...	14.427	5.7	ng	274588	5	14.151	967004	20.0
2,5,8,11,14-Pen...	15.374	2.5	ng	104175	6	15.680	837722	20.0
Benzo[e]pyrene	15.539	2.4	ng	98527	6	15.680	837722	20.0