LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138410.D
Acq On : 01 Jul 2024 18:36
Operator : CG\JU
Sample : P3077-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1-S-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: BF138410.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	10	16	21	rVB	2075012	2556015	75.80%	8.687%
2	2.287	30	34	45	rVB2	37711	59868	1.78%	0.203%
3	3.399	215	223	240	rBV3	103264	258048	7.65%	0.877%
4	5.098	508	512	521	rVB	290686	351039	10.41%	1.193%
5	5.363	553	557	561	rBV	56463	54064	1.60%	0.184%
6	5.469	571	575	577	rBV	277241	279761	8.30%	0.951%
7	5.504	577	581	584	rVB	3557262	3261714	96.73%	11.085%
8	5.722	615	618	622	rVB	365977	312563	9.27%	1.062%
9	5.822	631	635	640	rVB	44334	40670	1.21%	0.138%
10	6.510	747	752	755	rBV	3709184	3371848	100.00%	11.459%
11	6.698	781	784	788	rBV	94414	80353	2.38%	0.273%
12	6.875	810	814	817	rBV	1534995	1286480	38.15%	4.372%
13	6.934	820	824	827	rBV	45533	38280	1.14%	0.130%
14	7.010	834	837	842	rBV	112702	88946	2.64%	0.302%
15	7.434	904	909	912	rBV	2441278	2175415	64.52%	7.393%
16	7.687	948	952	960	rVB	151716	119639	3.55%	0.407%
17	8.151	1028	1031	1034	rBV	1835590	1597114	47.37%	5.428%
18	8.369	1063	1068	1074	rVB	48750	43267	1.28%	0.147%
19	8.463	1080	1084	1088	rBV	234755	186116	5.52%	0.633%
20	8.863	1149	1152	1155	rBV	127539	91323	2.71%	0.310%
21	8.963	1166	1169	1172	rVB	73207	56577	1.68%	0.192%
22	9.228	1210	1214	1217	rBV	3724690	2928685	86.86%	9.953%
23	9.304	1224	1227	1229	rBV	50673	38604	1.14%	0.131%
24	9.904	1326	1329	1333	rVB	1853516	1503870	44.60%	5.111%
25	10.004	1341	1346	1348	rBV2	105418	136103	4.04%	0.463%
26	10.592	1443	1446	1450	rBV2	29247	38280	1.14%	0.130%
27	10.633	1450	1453	1457	rVB	188920	143805	4.26%	0.489%
28	10.692	1459	1463	1466	rBV	1916891	1575597	46.73%	5.355%
29	10.804	1479	1482	1488	rVB2	35462	48132	1.43%	0.164%
30	11.392	1578	1582	1584	rBV	1367558	1158841	34.37%	3.938%
31	11.416	1584	1586	1589	rVV	183706	151655	4.50%	0.515%
32	11.463	1589	1594	1597	rVB	57019	56812	1.68%	0.193%
33	11.916	1668	1671	1677	rBV2	128113	132585	3.93%	0.451%
34	12.004	1683	1686	1688	rBV	41665	41899	1.24%	0.142%
35	12.598	1784	1787	1790	rBV	319985	258976	7.68%	0.880%
36	12.698	1801	1804	1808	rBV3	38288	47376	1.41%	0.161%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138410.D
Acq On : 01 Jul 2024 18:36
Operator : CG\JU
Sample : P3077-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-S-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	12.827	1821	1826	1832	rBV	288807	300123	8.90%	1.020%
38	12.974	1847	1851	1854	rBV	2248856	1922389	57.01%	6.533%
39	13.157	1879	1882	1884	rVB2	40523	37732	1.12%	0.128%
40	13.869	1999	2003	2008	rBV	171443	197204	5.85%	0.670%
41	14.027	2025	2030	2032	rBV	1155353	1162690	34.48%	3.951%
42	14.051	2032	2034	2040	rVB	137849	129898	3.85%	0.441%
43	14.492	2107	2109	2114	rBV4	56519	74920	2.22%	0.255%
44	14.798	2159	2161	2164	rBV2	41908	41621	1.23%	0.141%
45	15.063	2203	2206	2209	rBV	92667	127842	3.79%	0.434%
46	15.427	2265	2268	2274	rVB	72173	92822	2.75%	0.315%
47	15.492	2275	2279	2283	rBV	650323	767339	22.76%	2.608%

Sum of corrected areas: 29424900

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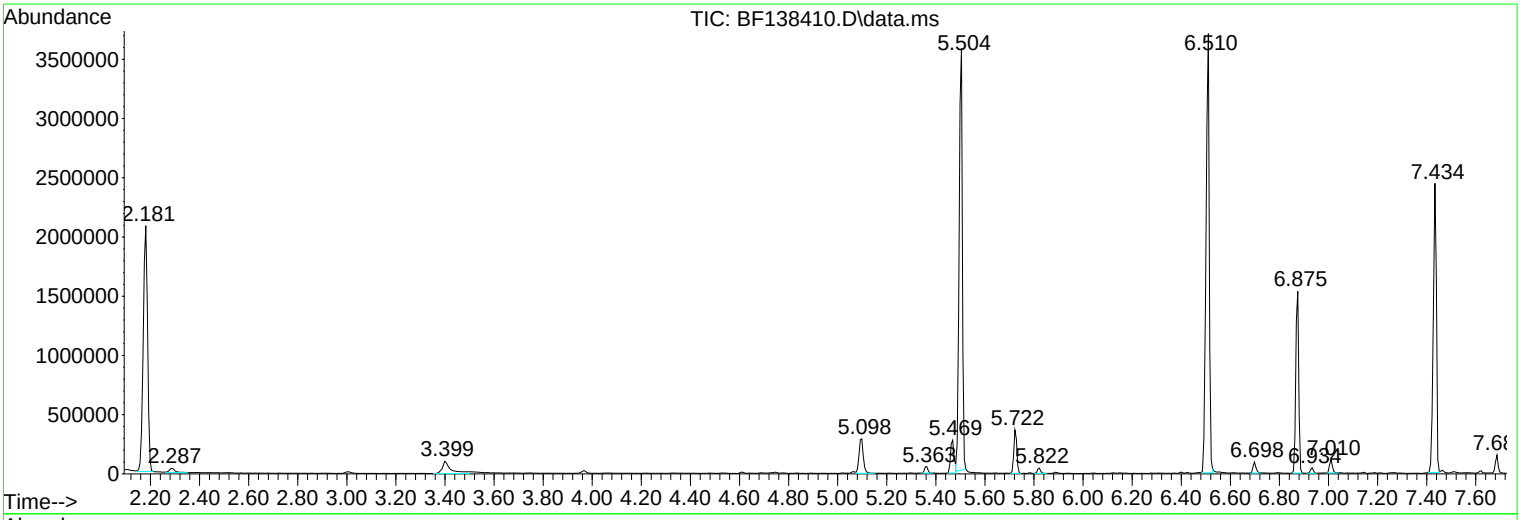
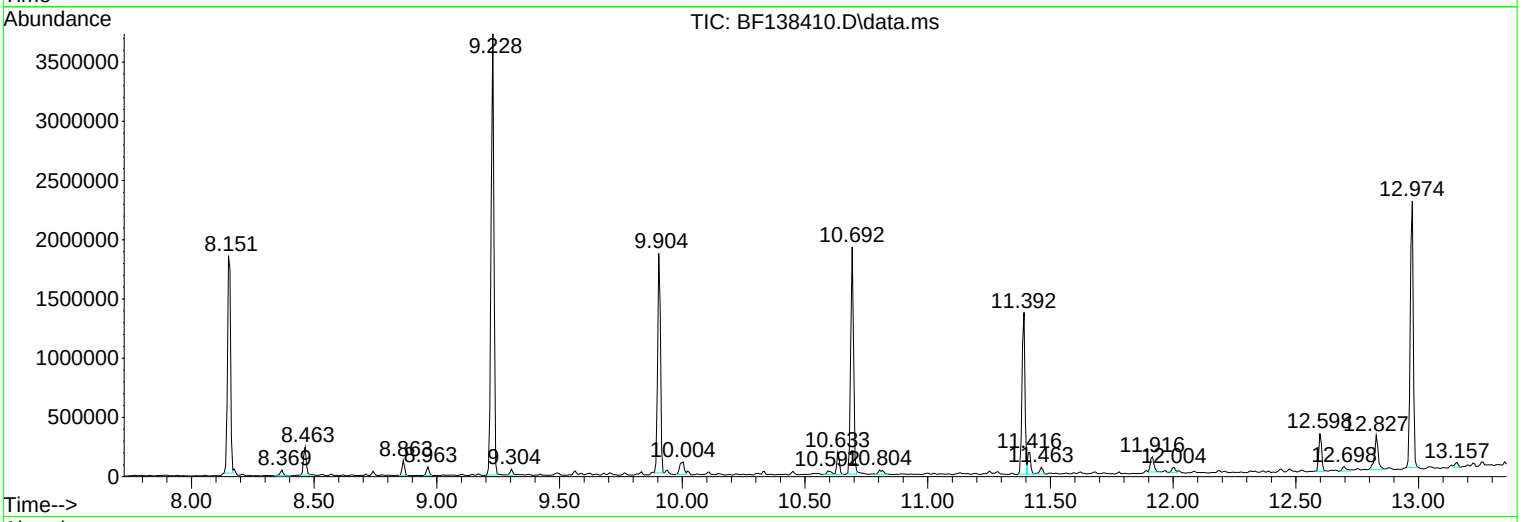
ALS Vial : 17 Sample Multiplier: 1

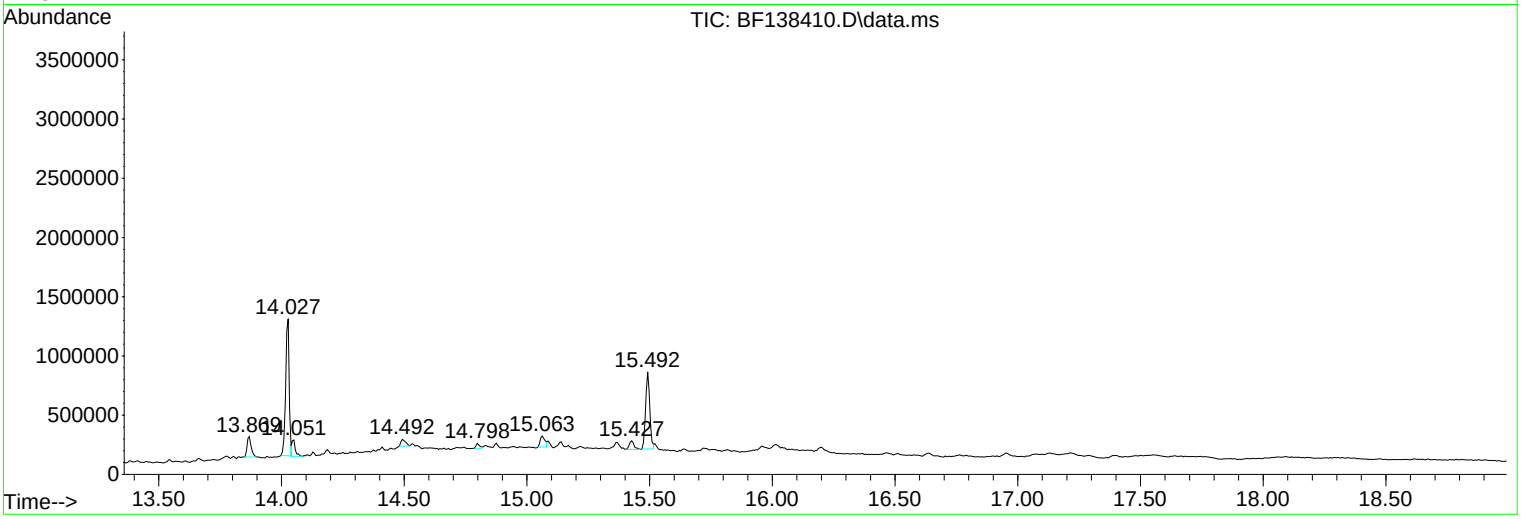
Instrument :
BNA_F
ClientSampleId :
1-S-1

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138410.D
Acq On : 01 Jul 2024 18:36
Operator : CG\JU
Sample : P3077-07
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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

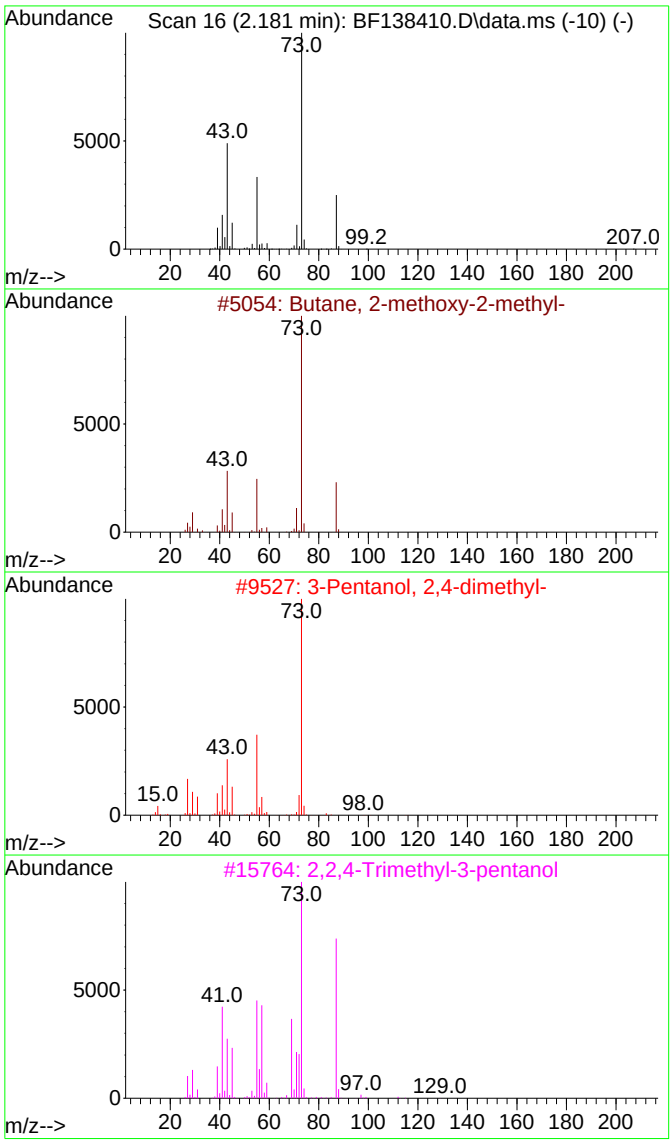
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

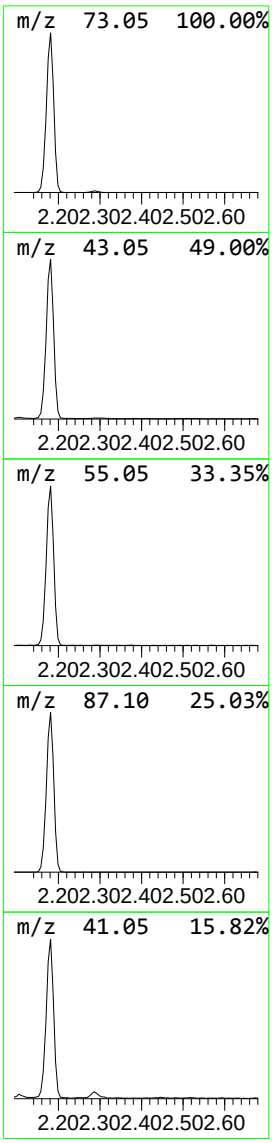
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	39.74 ng	2556020	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





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138410.D
Acq On : 01 Jul 2024 18:36
Operator : CG\JU
Sample : P3077-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-S-1

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

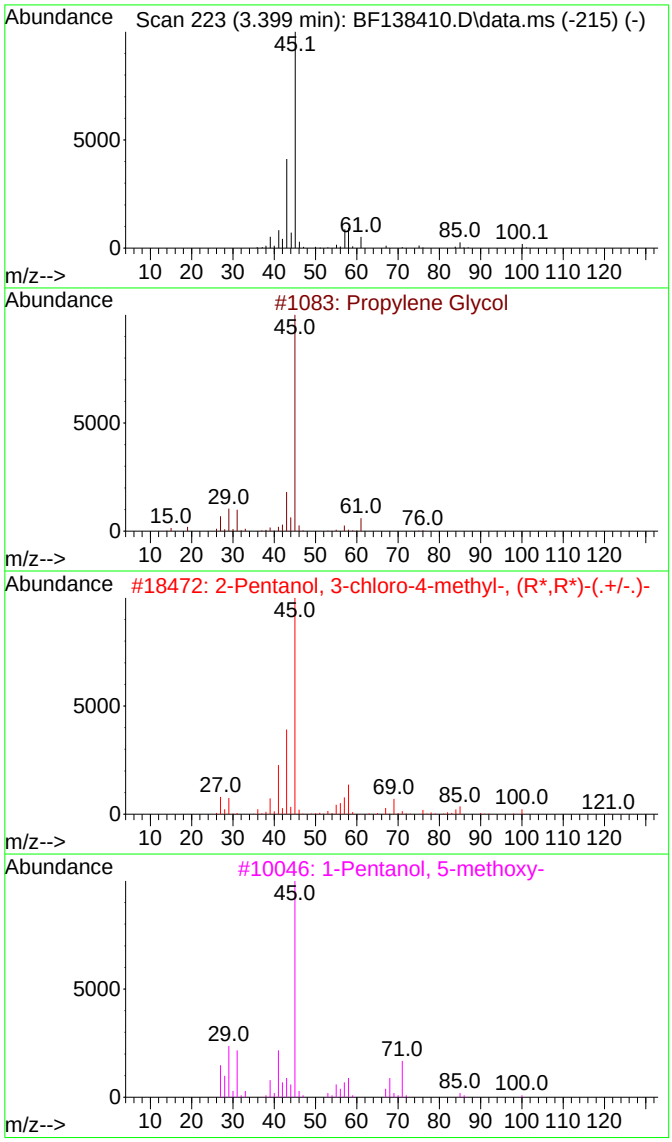
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

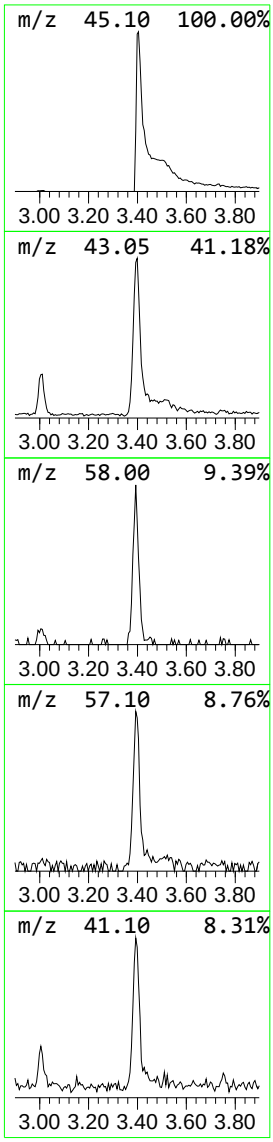
****

Peak Number 2 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.399	4.01 ng	258048	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	64
2	2-Pentanol, 3-chloro-4-methyl-, ...	136	C6H13ClO	074685-47-5	40
3	1-Pentanol, 5-methoxy-	118	C6H14O2	004799-62-6	40
4	2,3-Butanediol	90	C4H10O2	000513-85-9	38
5	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF070124\
Data File : BF138410.D
Acq On : 01 Jul 2024 18:36
Operator : CG\JU
Sample : P3077-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-S-1

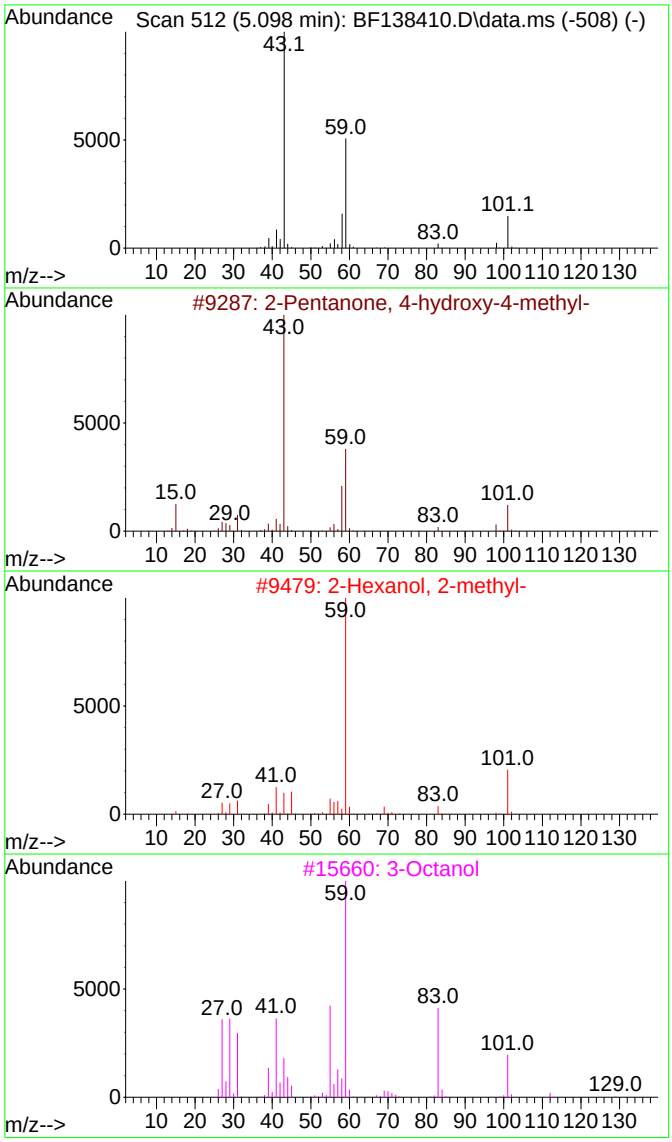
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

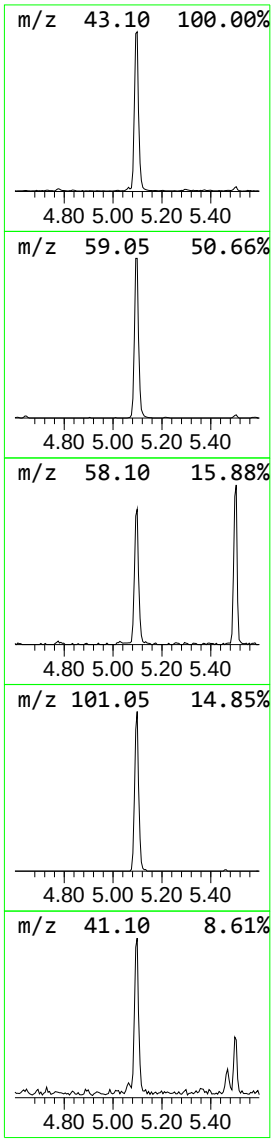
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	5.46 ng	351039	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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Octanol	130	C8H18O	000589-98-0	33
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-S-1

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

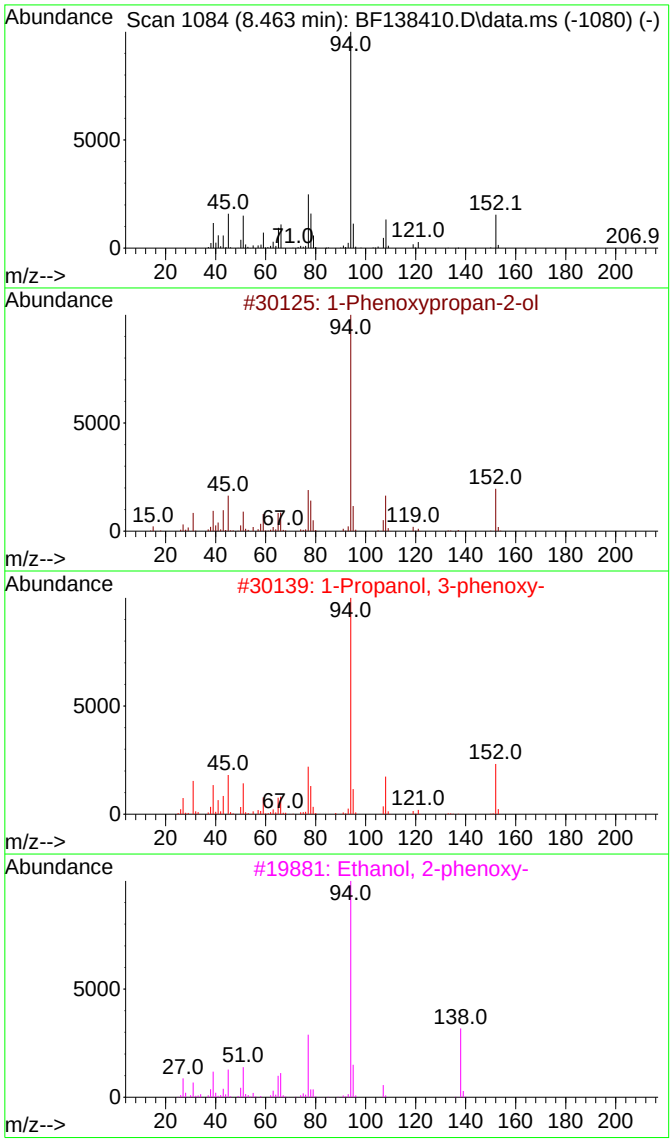
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

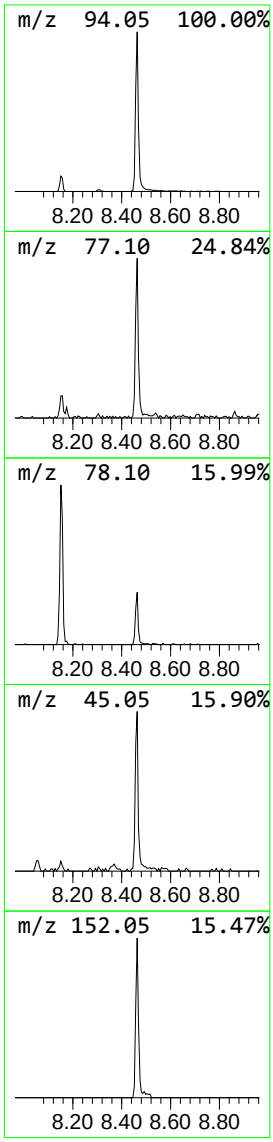
****

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.463	2.33 ng	186116	Naphthalene-d8	8.151

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	87
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5	Benzene, propoxy-	136	C9H12O	000622-85-5	53





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Instrument :
BNA_F
ClientSampleId :
1-S-1

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

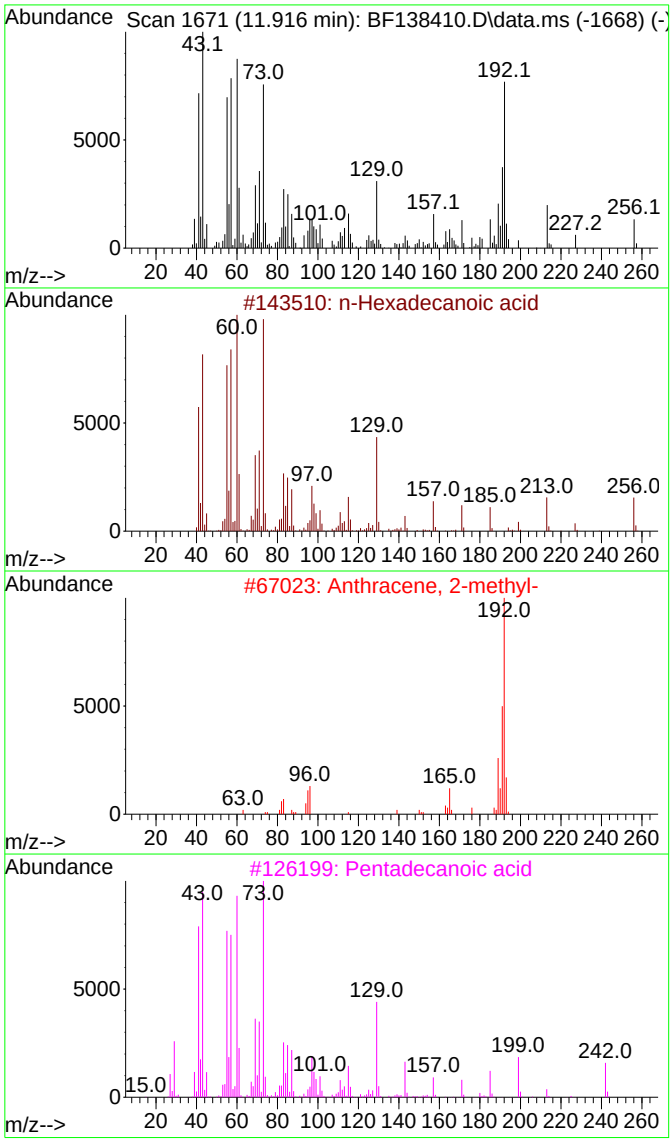
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

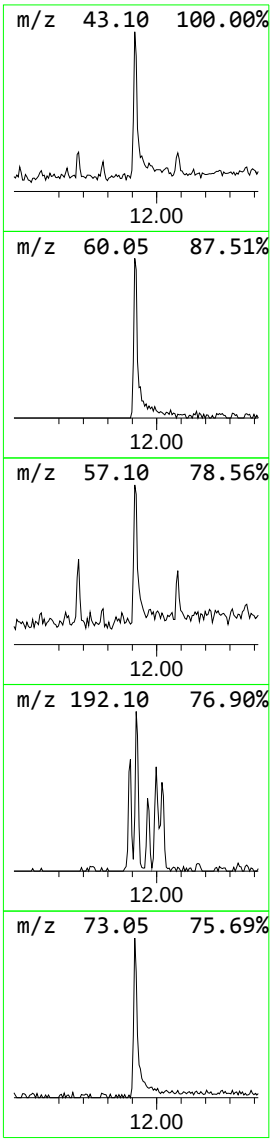
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.29 ng	132585	Phenanthrene-d10	11.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	46
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	46
4	n-Decanoic acid	172	C10H20O2	000334-48-5	42
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	35





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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

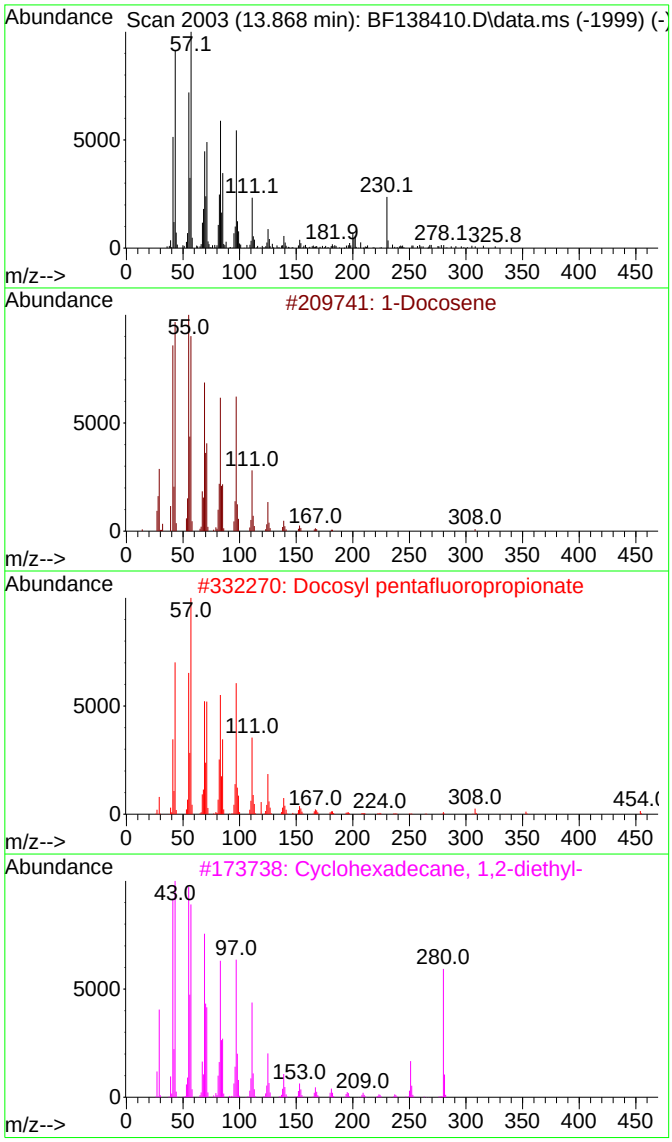
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

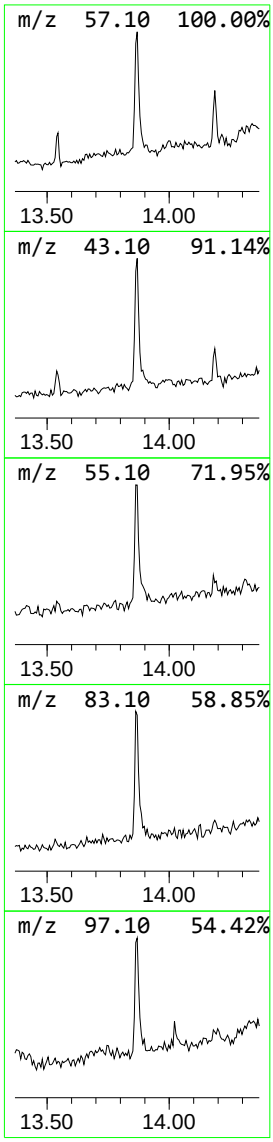
****

Peak Number 7 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	3.39 ng	197204	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	98
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
3	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	90
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	90
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87





Tentatively Identified Compound (LSC) summary

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Data File : BF138410.D
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Misc :
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.181	39.7	ng	2556020	1	6.875	1286480	20.0
Propylene Glycol	3.399	4.0	ng	258048	1	6.875	1286480	20.0
2-Pentanone, 4-...	5.098	5.5	ng	351039	1	6.875	1286480	20.0
1-Phenoxypropan...	8.463	2.3	ng	186116	2	8.151	1597110	20.0
n-Hexadecanoic ...	11.916	2.3	ng	132585	4	11.392	1158840	20.0
1-Docosene	13.868	3.4	ng	197204	5	14.027	1162690	20.0