LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112120\
Data File : BP004045.D
Acq On : 21 Nov 2020 19:13
Operator : CG/JU
Sample : L4839-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : B4-GW

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_P\METHODS\8270E-BP110320.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004045.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.917	3	5	25	rVB	1960577	2199304	30.21%	6.304%
2	3.076	26	32	41	rVB2	78780	149886	2.06%	0.430%
3	3.164	42	47	54	rBV	532728	665118	9.14%	1.907%
4	5.264	399	404	413	rVB	85018	122067	1.68%	0.350%
5	5.805	488	496	514	rBV	1341550	2109059	28.97%	6.045%
6	7.452	767	776	789	rBV	982053	1663180	22.85%	4.767%
7	8.263	907	914	923	rBV	402344	641696	8.82%	1.839%
8	9.428	1104	1112	1124	rBV	1514038	2534837	34.82%	7.266%
9	11.093	1387	1395	1407	rBV	506588	851842	11.70%	2.442%
10	13.510	1799	1806	1819	rBV	3674552	5286376	72.62%	15.153%
11	14.310	1936	1942	1953	rBV	131354	188272	2.59%	0.540%
12	14.887	2033	2040	2049	rBV2	748919	1067194	14.66%	3.059%
13	16.375	2286	2293	2313	rBV	2654118	4064584	55.84%	11.651%
14	17.622	2498	2505	2511	rBV	852986	1219470	16.75%	3.496%
15	18.469	2644	2649	2674	rBV	572140	1229805	16.89%	3.525%
16	18.892	2717	2721	2729	rBV	78254	111811	1.54%	0.320%
17	19.675	2850	2854	2863	rBV	199793	328492	4.51%	0.942%
18	20.122	2924	2930	2935	rBV	5699605	7279401	100.00%	20.866%
19	21.310	3128	3132	3141	rBV	262485	469967	6.46%	1.347%
20	21.651	3185	3190	3196	rBV	1033531	1318721	18.12%	3.780%
21	24.121	3603	3610	3621	rVB2	687371	1385682	19.04%	3.972%

Sum of corrected areas: 34886764

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112120\
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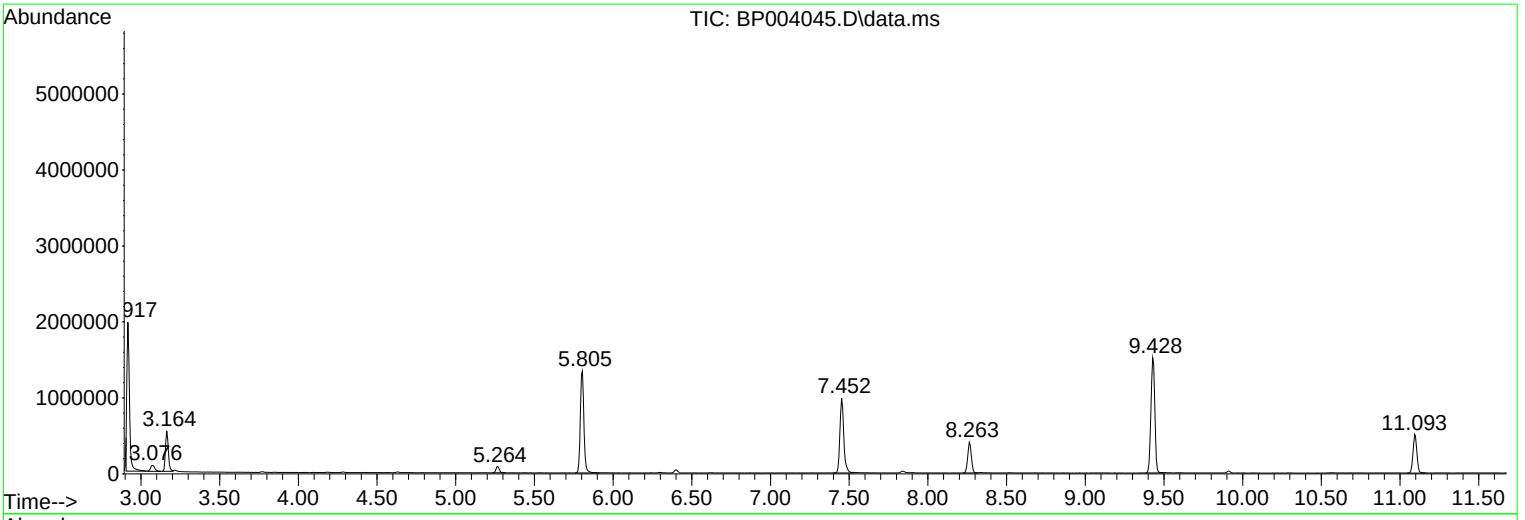
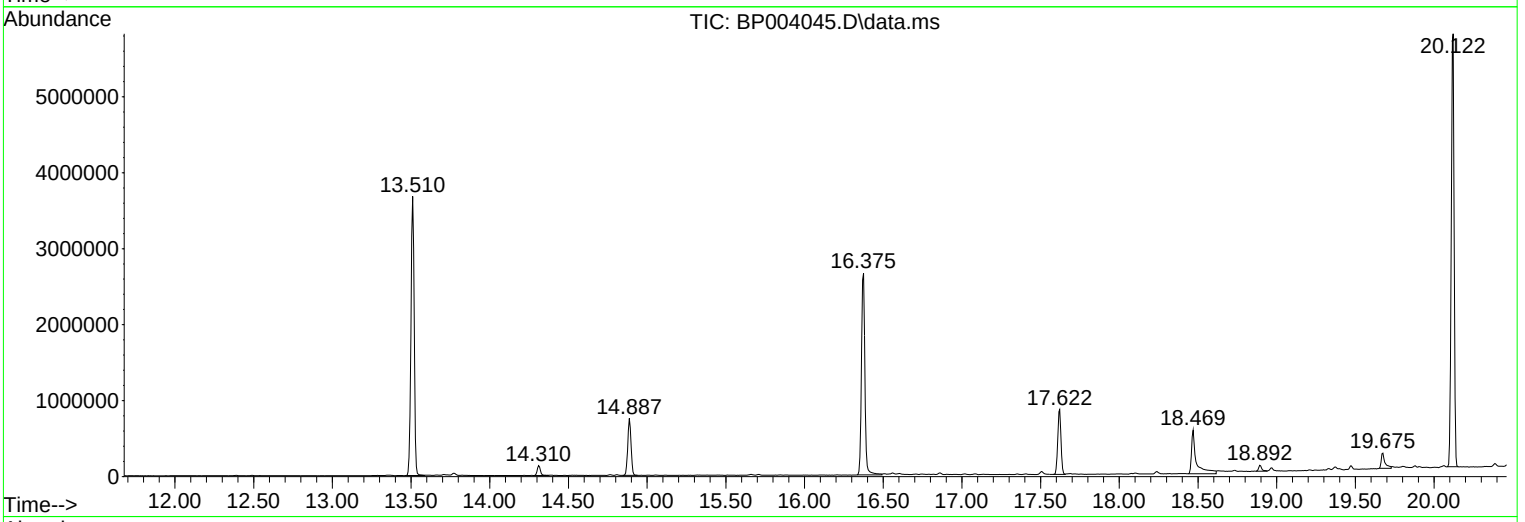
Misc :
ALS Vial : 9 Sample Multiplier: 1

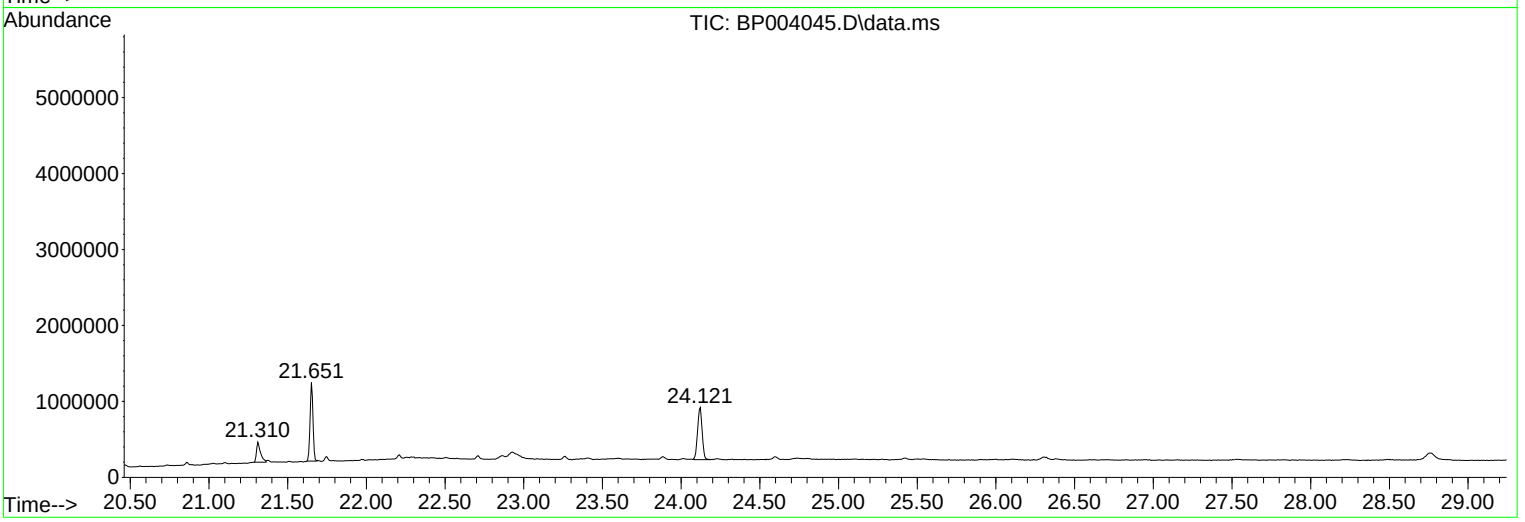
Instrument :
BNA_P
ClientSampleId :
B4-GW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

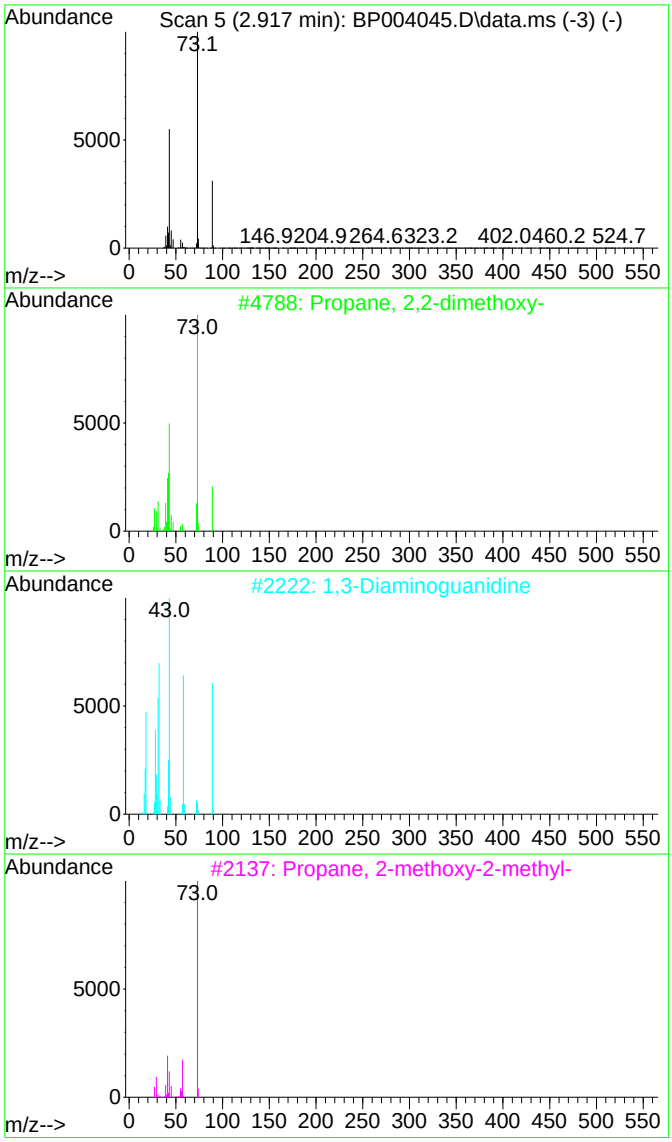
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

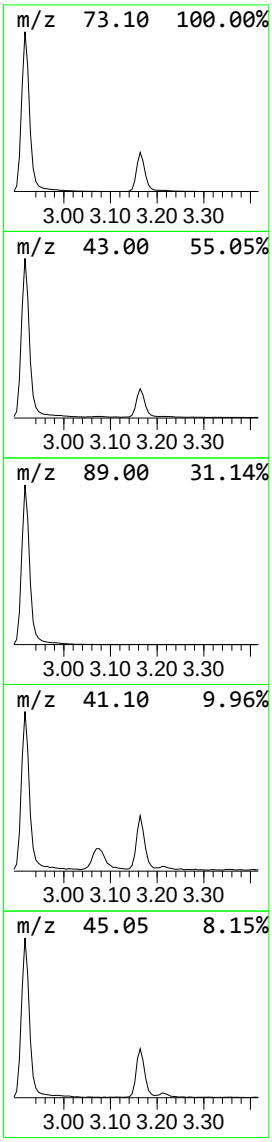
****

Peak Number 1 unknown2.917 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.917	68.55 ng	2199300	1,4-Dichlorobenzene-d4	8.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Sample : L4839-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B4-GW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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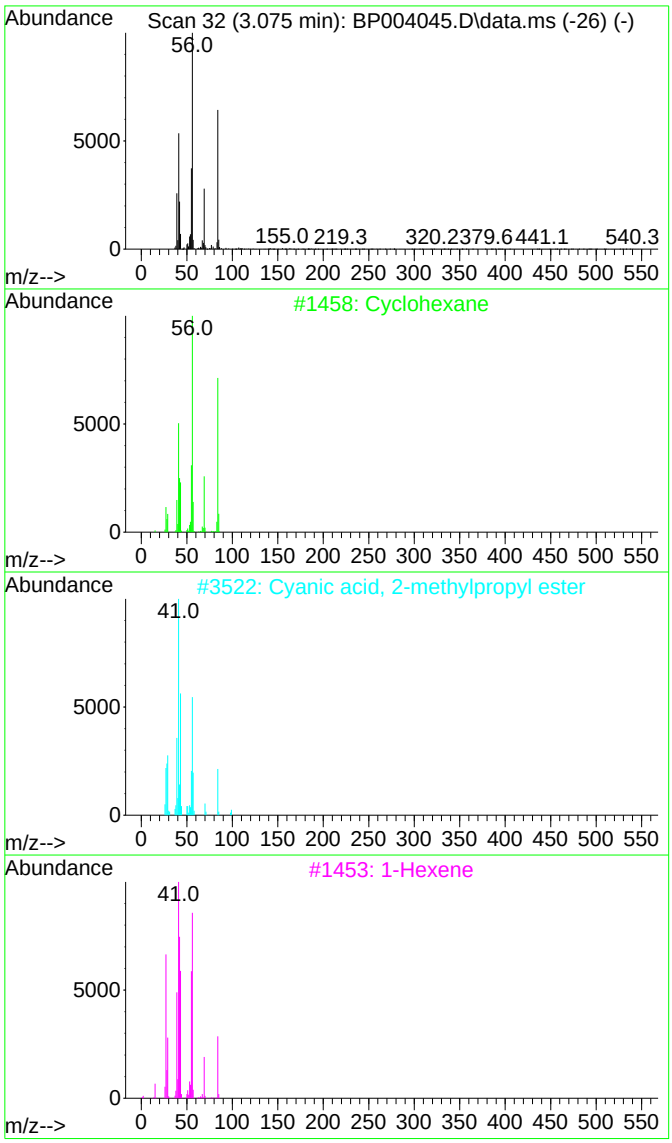
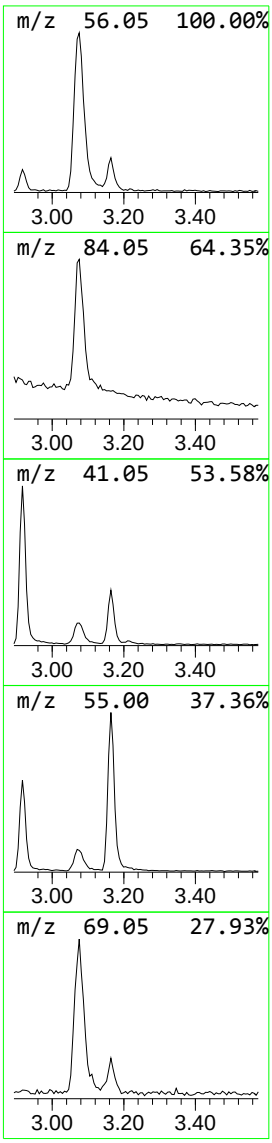
Peak Number 2 Cyclohexane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.075	4.67 ng	149886	1,4-Dichlorobenzene-d4	8.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	91
2	Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	64
3	1-Hexene	84	C6H12	000592-41-6	59
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	56
5	Cyclobutane	56	C4H8	000287-23-0	46





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Data File : BP004045.D
Acq On : 21 Nov 2020 19:13
Operator : CG/JU
Sample : L4839-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B4-GW

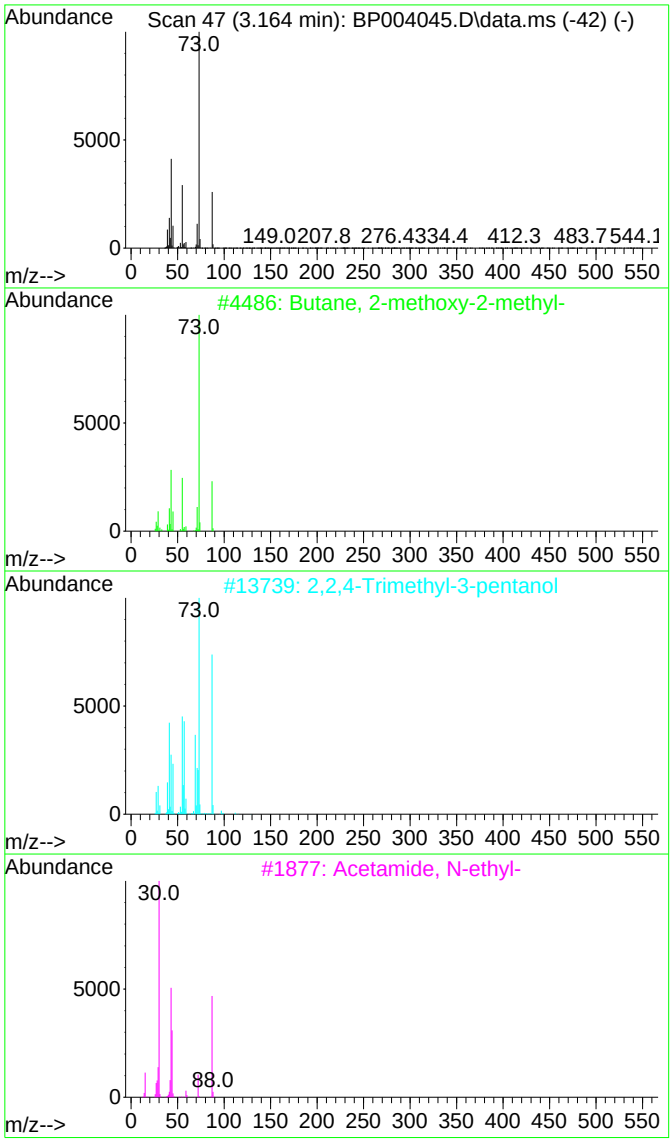
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

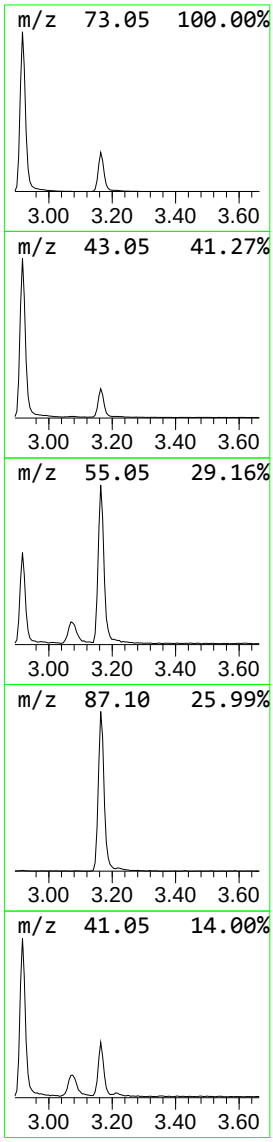
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.164	20.73 ng	665118	1,4-Dichlorobenzene-d4	8.263

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 : L4839-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B4-GW

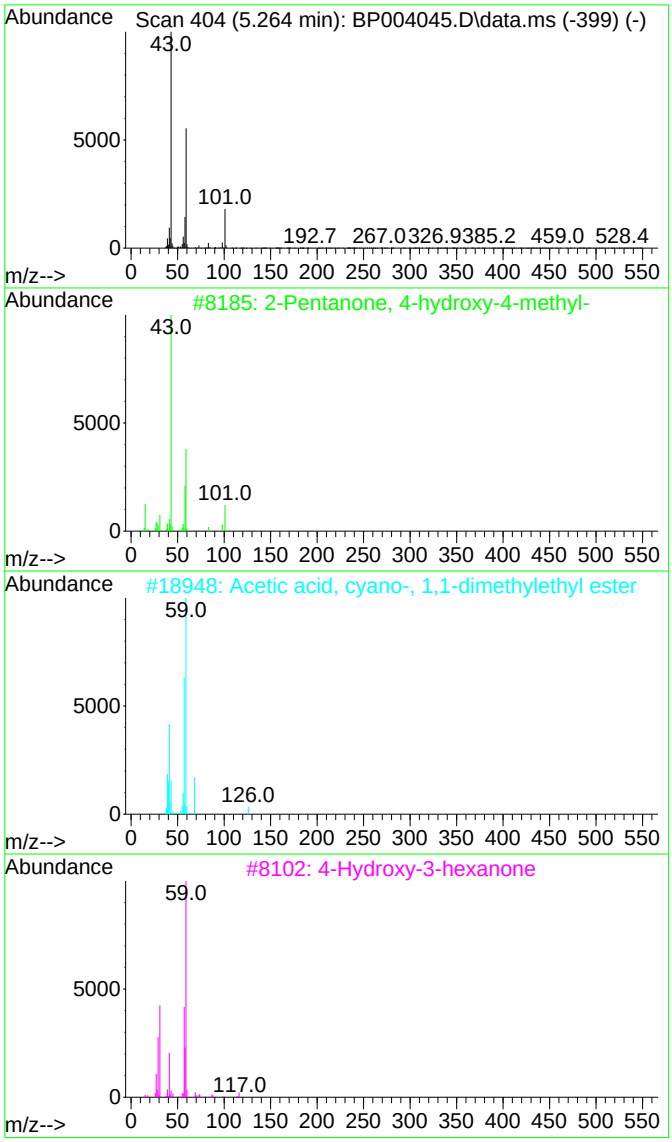
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

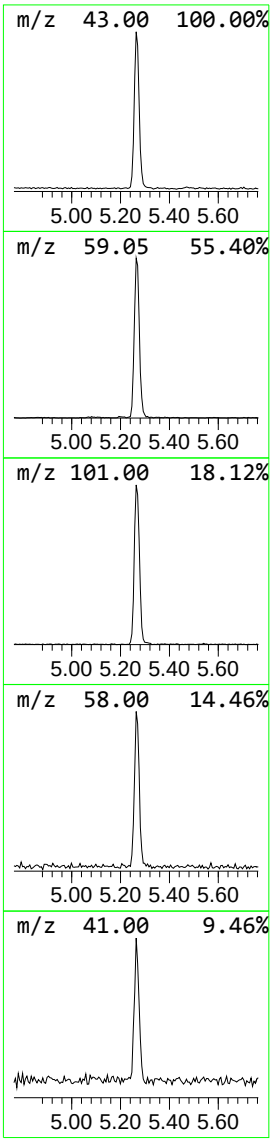
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.264	3.80 ng	122067	1,4-Dichlorobenzene-d4	8.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Operator : CG/JU
Sample : L4839-06
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : B4-GW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

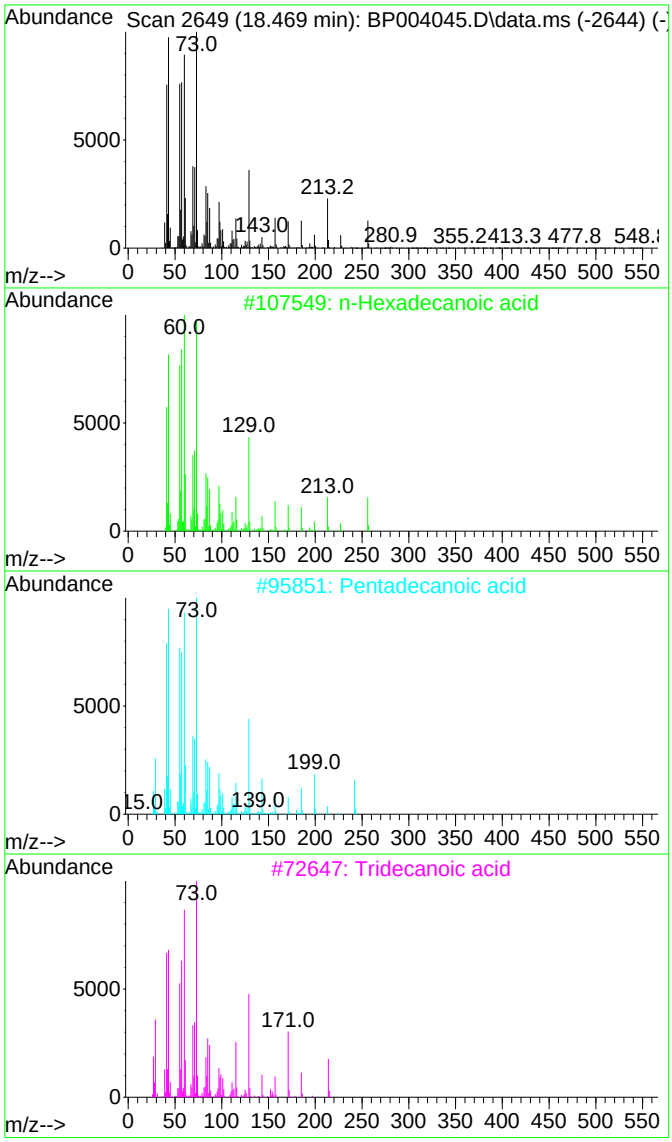
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

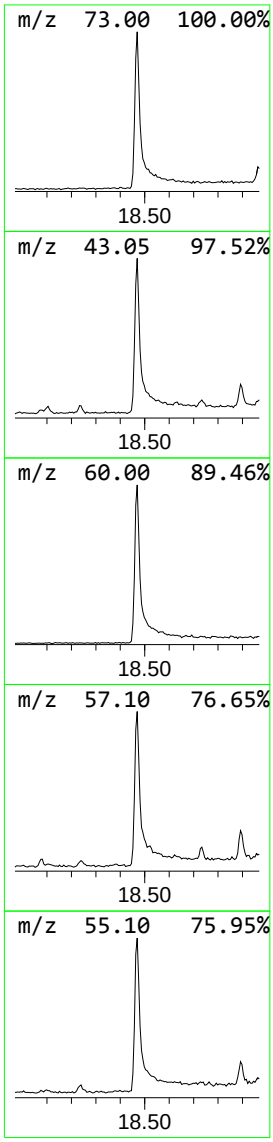
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.469	20.17 ng	1229810	Phenanthrene-d10	17.622

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Octadecanoic acid	284	C18H36O2	000057-11-4	91
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	90





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ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : B4-GW

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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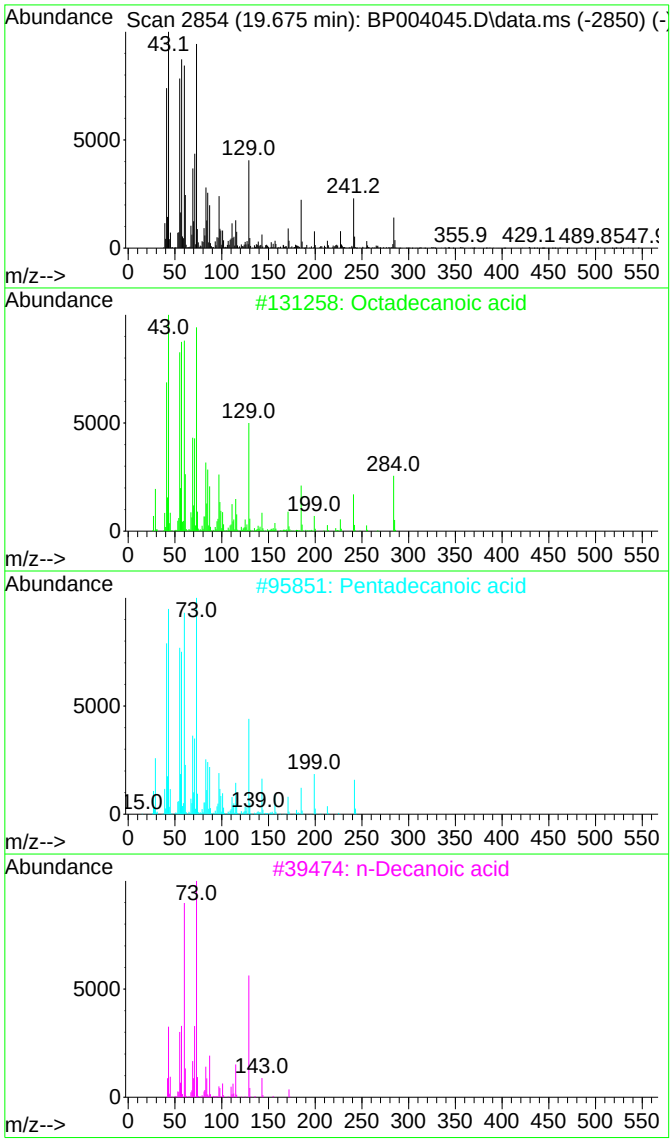
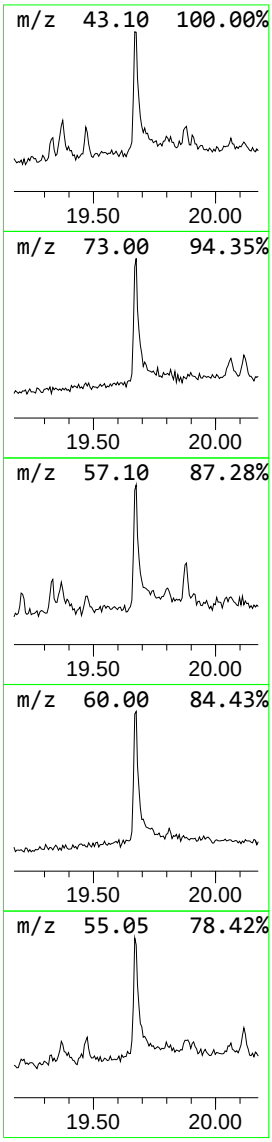
****

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.675	4.98 ng	328492	Chrysene-d12	21.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Decanoic acid	172	C10H20O2	000334-48-5	91
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86





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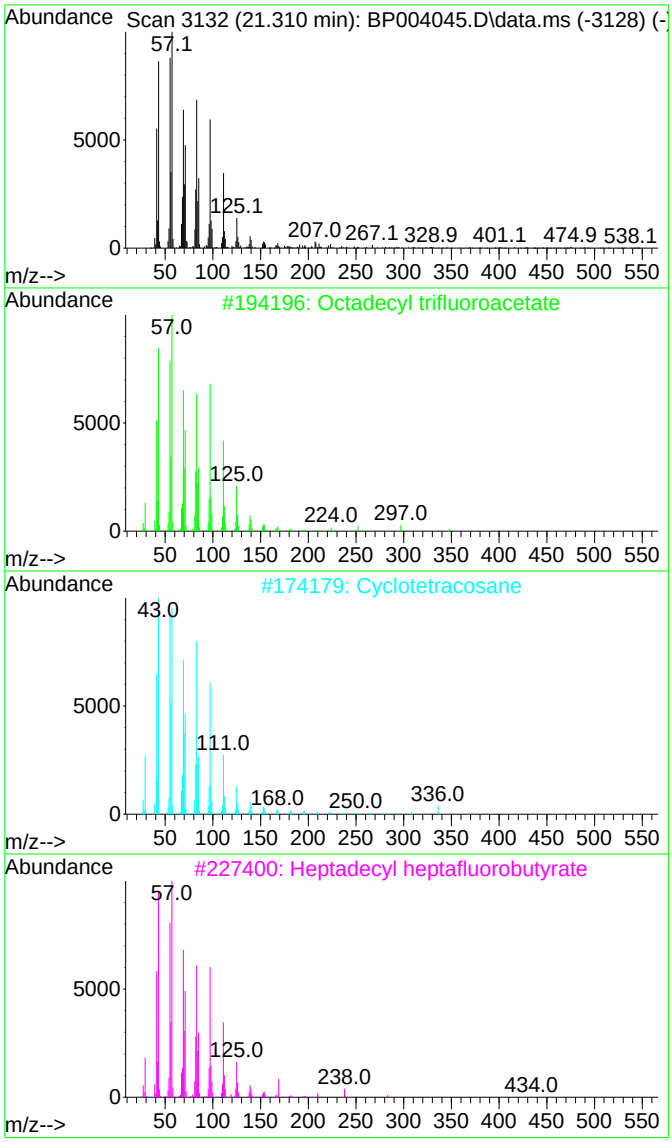
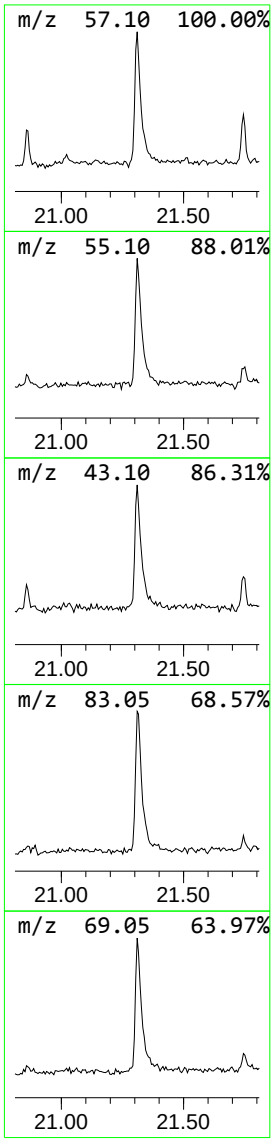
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Octadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.310	7.13 ng	469967	Chrysene-d12	21.651

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
2	Cyclotetracosane	336	C24H48	000297-03-0	94
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.917	2.917	68.5	ng	2199300	1	8.263	641696	20.0
Cyclohexane	3.075	4.7	ng	149886	1	8.263	641696	20.0
Butane, 2-metho...	3.164	20.7	ng	665118	1	8.263	641696	20.0
2-Pentanone, 4-...	5.264	3.8	ng	122067	1	8.263	641696	20.0
n-Hexadecanoic ...	18.469	20.2	ng	1229810	4	17.622	1219470	20.0
Octadecanoic acid	19.675	5.0	ng	328492	5	21.651	1318720	20.0
Octadecyl trifl...	21.310	7.1	ng	469967	5	21.651	1318720	20.0