LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070221\
Data File : BG049176.D
Acq On : 2 Jul 2021 20:54
Operator : CG/JU
Sample : M2900-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VB16208

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_G\METHODS\8270-BG063021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049176.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.126	9	15	25	rBV3	53938	133495	6.42%	1.058%
2	3.208	25	29	36	rVB2	21890	38028	1.83%	0.301%
3	3.825	129	134	139	rBV2	22874	33548	1.61%	0.266%
4	5.165	357	362	369	rBV	18514	29719	1.43%	0.235%
5	5.635	435	442	452	rBV	616507	1033154	49.72%	8.187%
6	7.239	707	715	726	rBV	685412	1221748	58.80%	9.681%
7	7.673	783	789	796	rBV2	14368	28292	1.36%	0.224%
8	8.085	852	859	867	rVB	128641	215953	10.39%	1.711%
9	9.254	1048	1058	1066	rBV	416477	759882	36.57%	6.021%
10	10.664	1291	1298	1309	rBV2	41252	78916	3.80%	0.625%
11	10.905	1331	1339	1349	rBV	171072	312527	15.04%	2.476%
12	13.349	1747	1755	1763	rBV	956446	1492578	71.83%	11.827%
13	13.614	1793	1800	1806	rBV	168356	263139	12.66%	2.085%
14	14.172	1889	1895	1902	rBV	121419	176011	8.47%	1.395%
15	14.730	1984	1990	1997	rVB	293971	458375	22.06%	3.632%
16	15.834	2173	2178	2190	rBV	174018	264373	12.72%	2.095%
17	16.216	2236	2243	2255	rBV	1074640	1659601	79.87%	13.151%
18	17.480	2451	2458	2464	rBV	385551	601942	28.97%	4.770%
19	18.361	2602	2608	2616	rBV4	25453	57729	2.78%	0.457%
20	19.213	2748	2753	2760	rBV2	52299	89202	4.29%	0.707%
21	19.530	2803	2807	2812	rVB	44504	53891	2.59%	0.427%
22	20.082	2895	2901	2910	rBV	1529985	2077967	100.00%	16.466%
23	20.353	2943	2947	2952	rBV6	17461	26559	1.28%	0.210%
24	21.387	3119	3123	3133	rBV4	69472	126187	6.07%	1.000%
25	21.639	3161	3166	3174	rBV7	28834	67919	3.27%	0.538%
26	21.763	3181	3187	3194	rVB	366070	636130	30.61%	5.041%
27	25.065	3739	3749	3765	rVB2	223959	683017	32.87%	5.412%

Sum of corrected areas: 12619882

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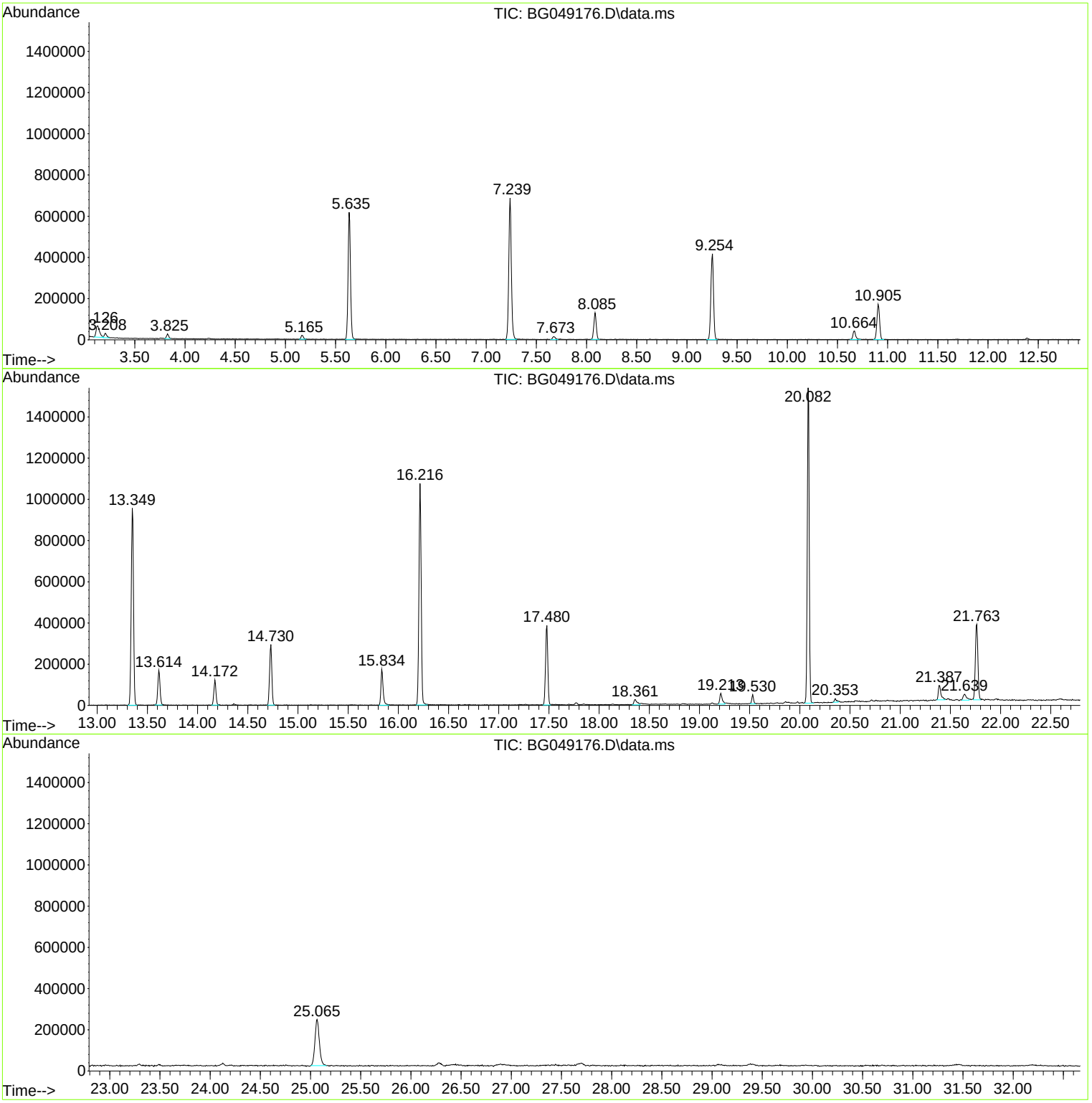
Instrument : BNA_G
ClientSampleId : VB16208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.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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Data File : BG049176.D
Acq On : 2 Jul 2021 20:54
Operator : CG/JU
Sample : M2900-01
Misc :
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Instrument : BNA_G
ClientSampleId : VB16208

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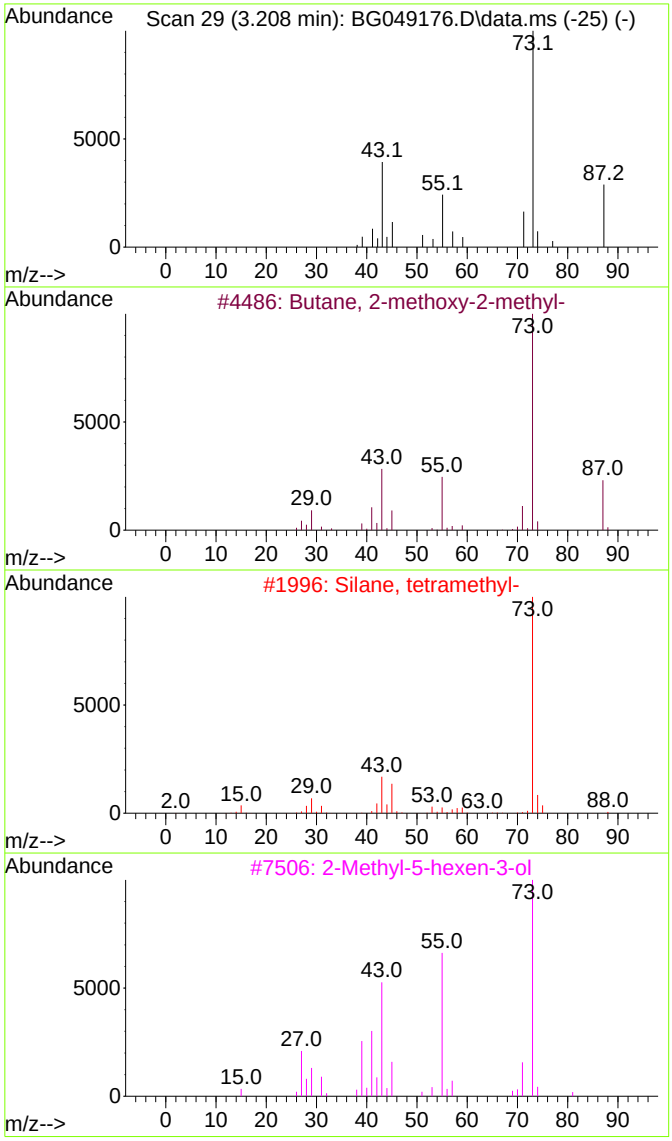
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

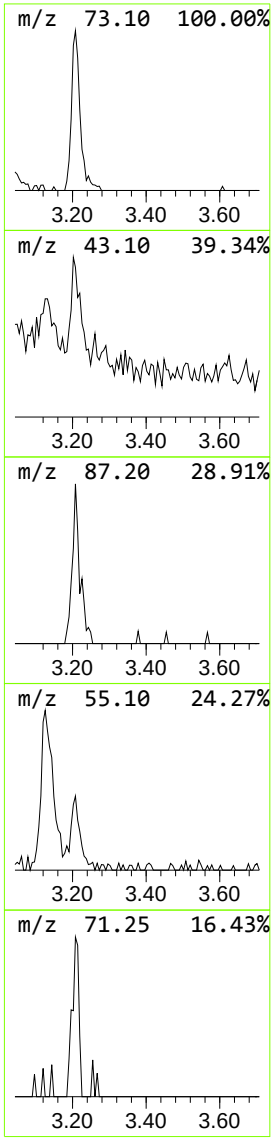
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.208	3.52 ng	38028	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	37
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	5
5	Isobutylamine	73	C4H11N	000078-81-9	4





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Data File : BG049176.D
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Operator : CG/JU
Sample : M2900-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VB16208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

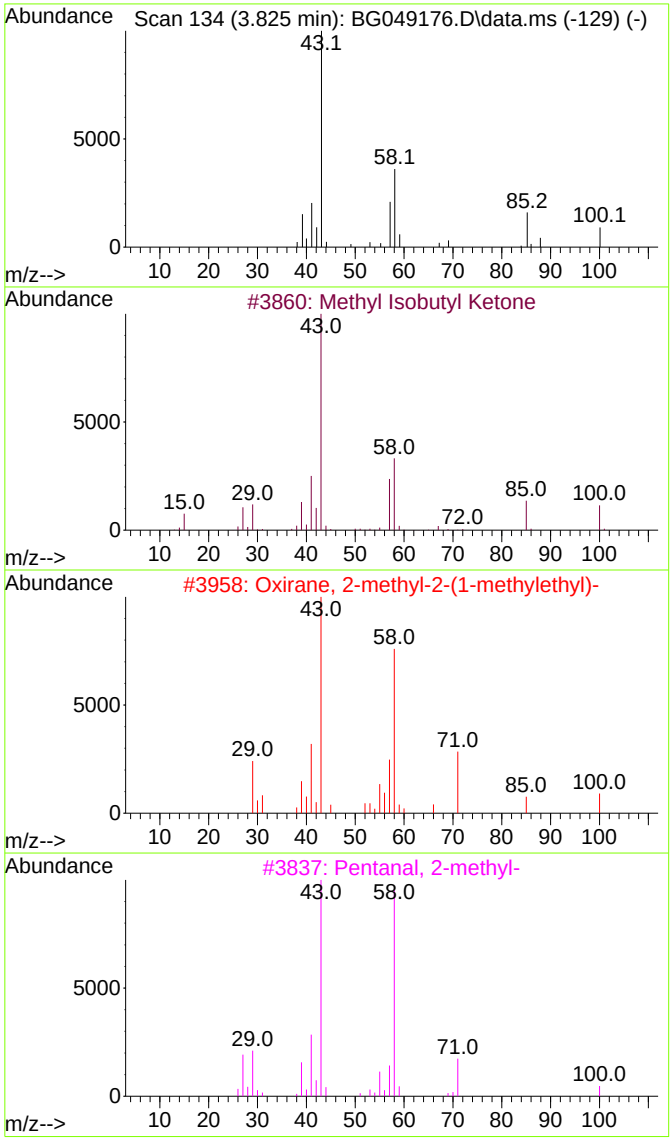
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

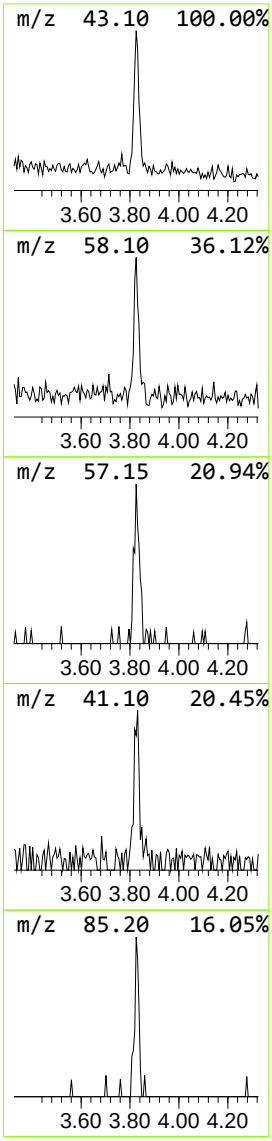
****

Peak Number 3 Methyl Isobutyl Ketone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.825	3.11 ng	33548	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	83
2	Oxirane, 2-methyl-2-(1-methyleth...	100	C6H12O	072221-03-5	38
3	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	37
4	2-Heptanone, 4-methyl-	128	C8H16O	006137-06-0	36
5	Octane	114	C8H18	000111-65-9	32





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Operator : CG/JU
Sample : M2900-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VB16208

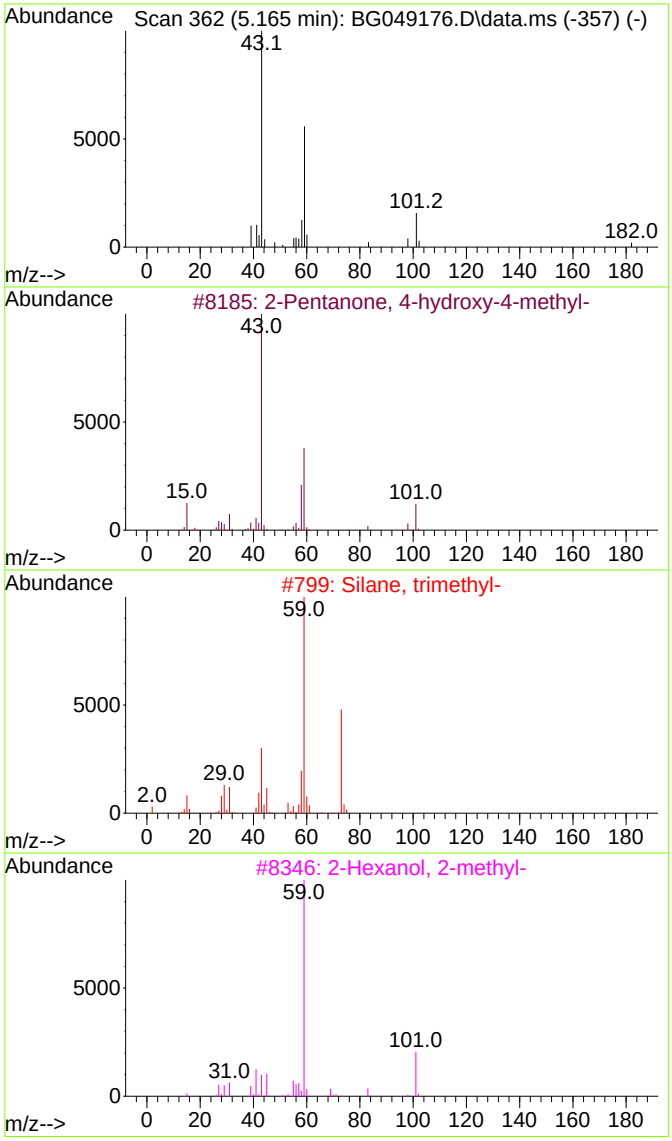
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

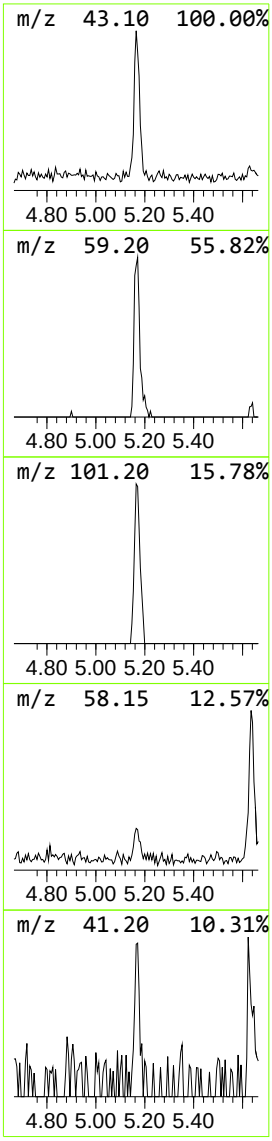
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.165	2.75 ng	29719	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Silane, trimethyl-	74	C3H10Si	000993-07-7	37
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4	Allyl dithioacetate	132	C5H8S2	027249-83-8	25
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	12





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Sample : M2900-01
Misc :
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Instrument : BNA_G
ClientSampleId : VB16208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

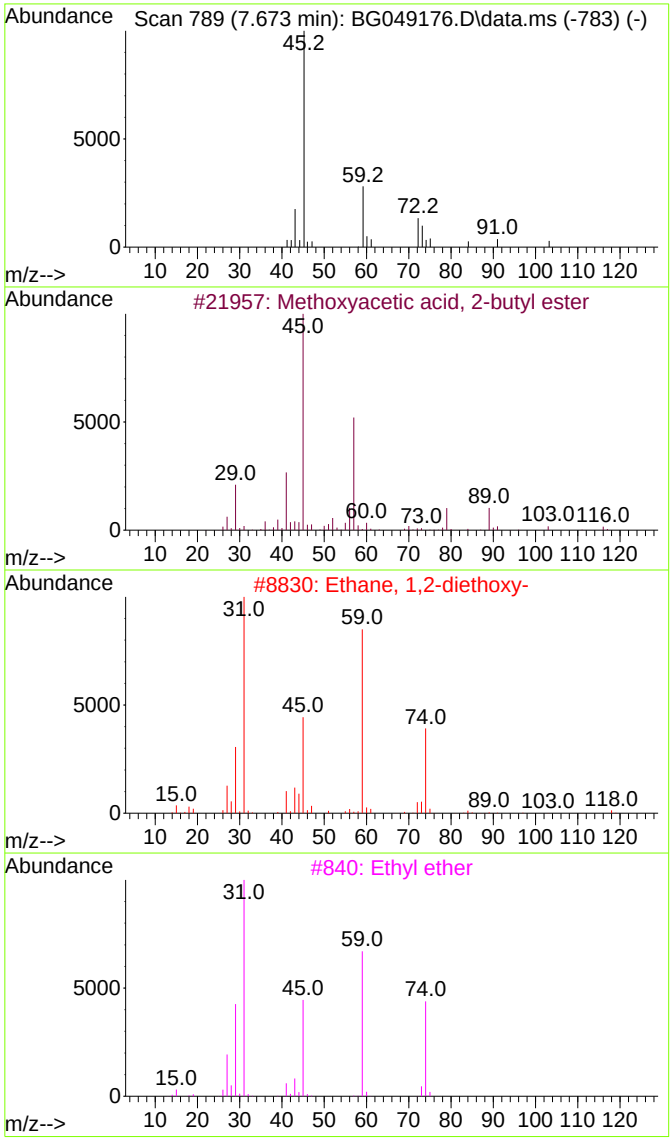
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

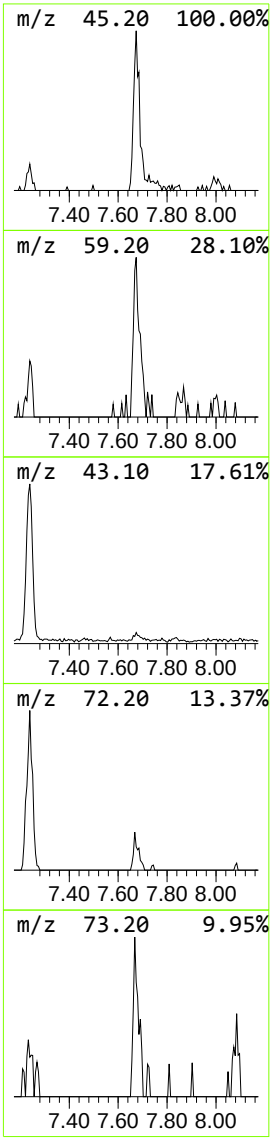
****

Peak Number 5 unknown7.673 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.673	2.62 ng	28292	1,4-Dichlorobenzene-d4	8.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	40
2	Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	38
3	Ethyl ether	74	C4H10O	000060-29-7	33
4	Methoxyacetic acid, 2-methylprop...	146	C7H14O3	1000282-40-9	33
5	Methoxyacetic acid, 2-pentyl ester	160	C8H16O3	1000282-69-2	9





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Operator : CG/JU
Sample : M2900-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : VB16208

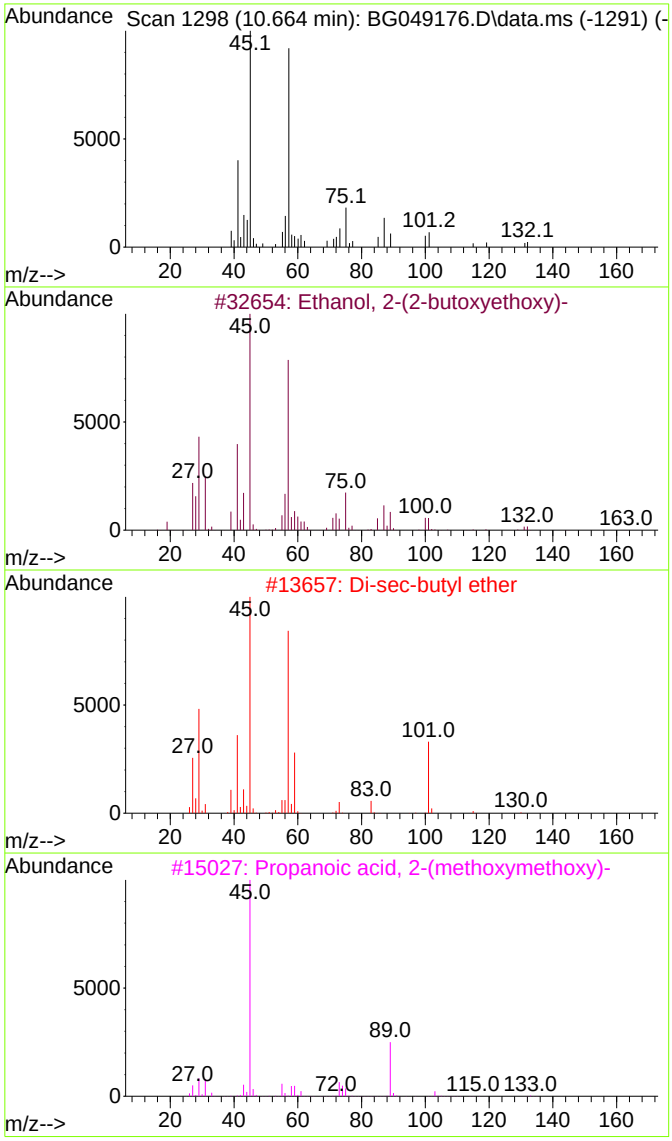
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

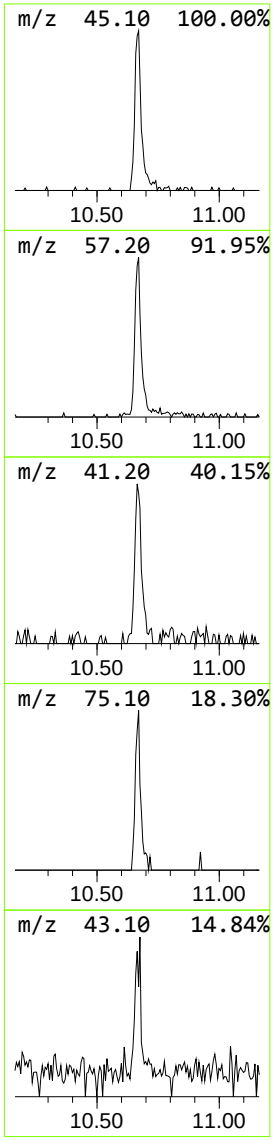
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.664	5.05 ng	78916	Naphthalene-d8	10.905

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
2	Di-sec-butyl ether	130	C8H18O	006863-58-7	59
3	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5	Hexane, 1-(methoxymethoxy)-	146	C8H18O2	066675-06-7	50





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Misc :
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Instrument : BNA_G
ClientSampleId : VB16208

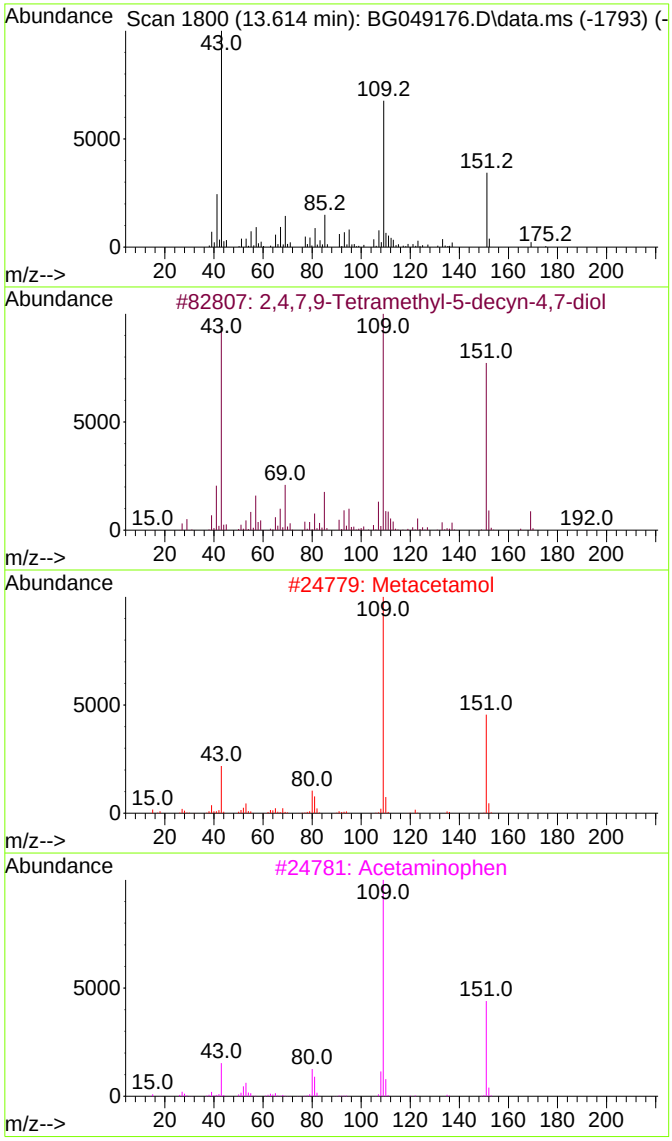
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

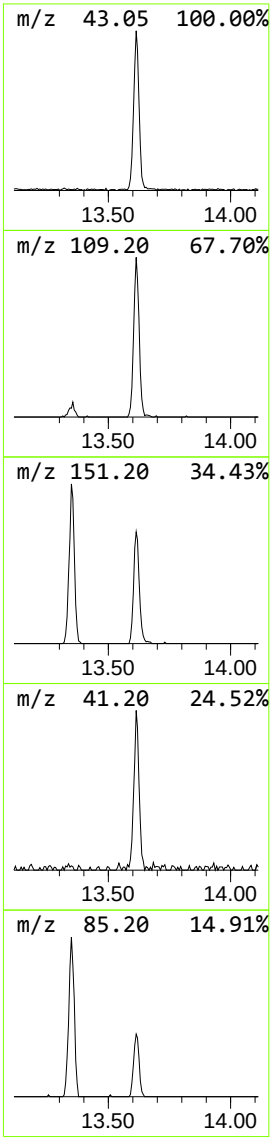
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.614	11.48 ng	263139	Acenaphthene-d10	14.730

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90
2	Metacetamol	151	C8H9NO2	000621-42-1	52
3	Acetaminophen	151	C8H9NO2	000103-90-2	52
4	Benzenamine, 4-propoxy-	151	C9H13NO	004469-80-1	50
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	50





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BNA_G
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VB16208

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

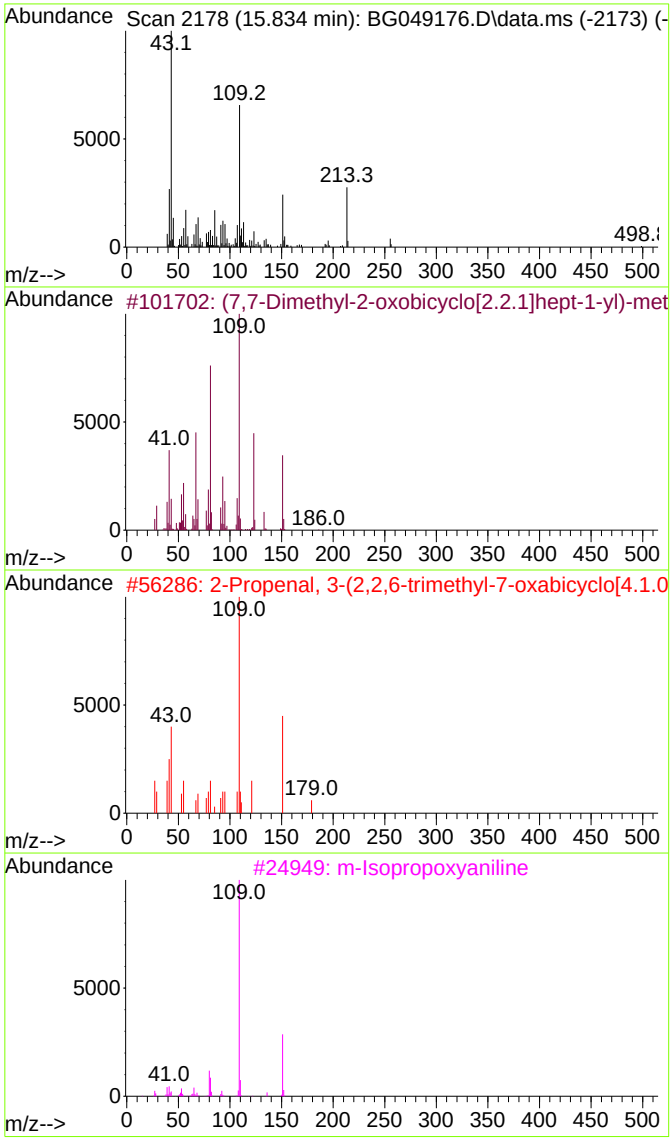
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

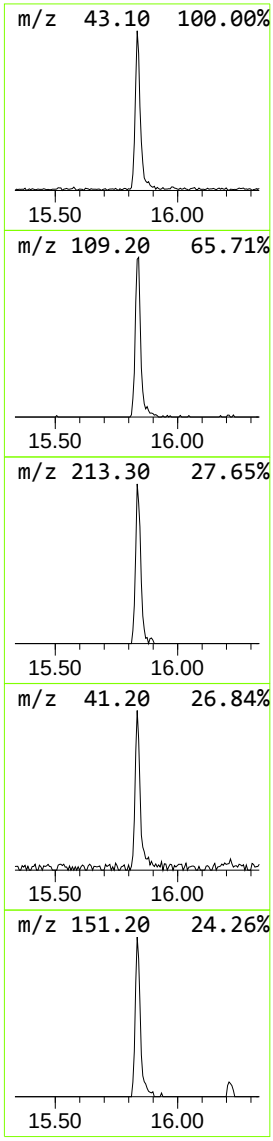
****

Peak Number 8 unknown15.834 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.834	11.54 ng	264373	Acenaphthene-d10	14.730

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(7,7-Dimethyl-2-oxobicyclo[2.2.1...	250	C10H15ClO3S	1000194-76-1	47
2	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	47
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	38
4	N-Cyclopropyl-p-fluorobenzylamine	165	C10H12FN	1000250-88-9	35
5	Acetaminophen	151	C8H9NO2	000103-90-2	35





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Misc :
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Instrument : BNA_G
ClientSampleId : VB16208

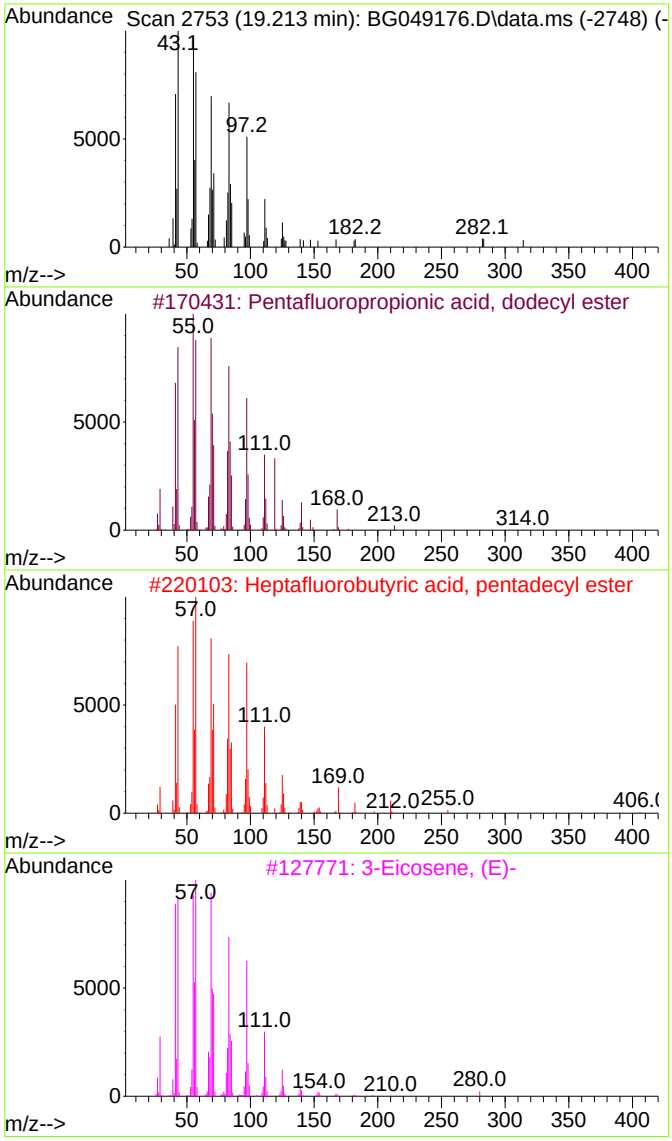
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

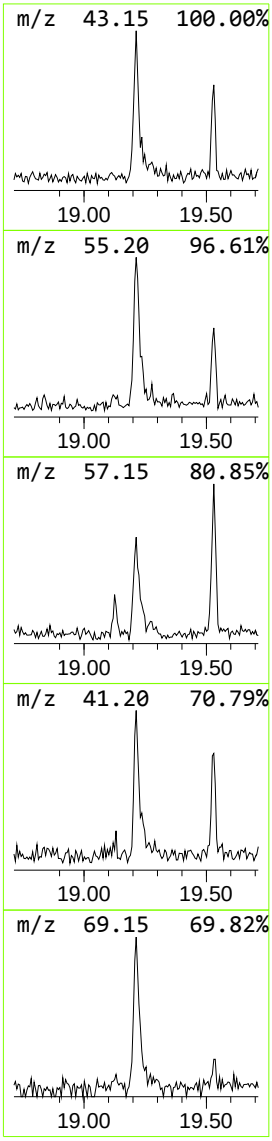
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.213	2.96 ng	89202	Phenanthrene-d10	17.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	91
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	87
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
5	1-Heneicosanol	312	C21H44O	015594-90-8	87





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Instrument :
BNA_G
ClientSampleId :
VB16208

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

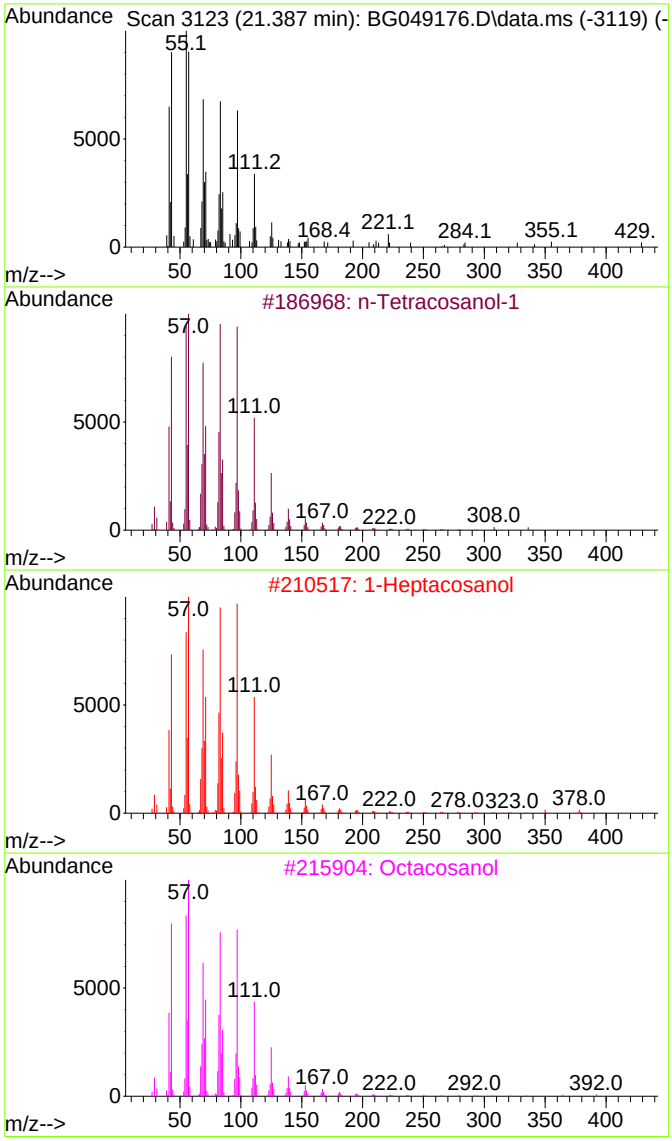
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

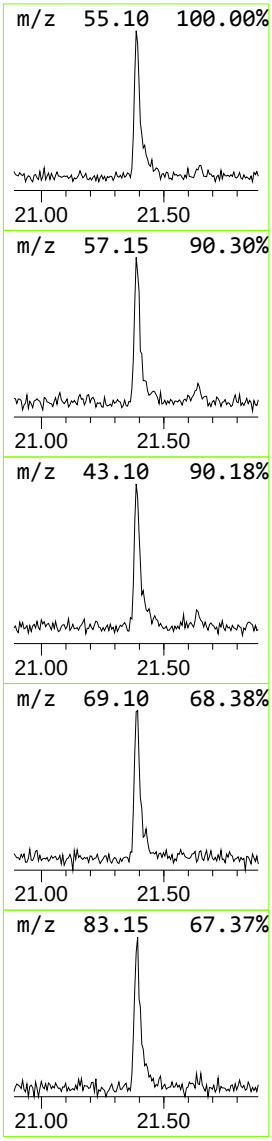
****

Peak Number 10 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.387	3.97 ng	126187	Chrysene-d12	21.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	1-Heptacosanol	396	C27H56O	002004-39-9	91
3	Octacosanol	410	C28H58O	000557-61-9	90
4	1-Docosene	308	C22H44	001599-67-3	87
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	86





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
Butane, 2-metho...	3.208	3.5	ng	38028	1	8.085	215953	20.0
Methyl Isobutyl...	3.825	3.1	ng	33548	1	8.085	215953	20.0
2-Pentanone, 4-...	5.165	2.8	ng	29719	1	8.085	215953	20.0
unknown7.673	7.673	2.6	ng	28292	1	8.085	215953	20.0
Ethanol, 2-(2-b...	10.664	5.0	ng	78916	2	10.905	312527	20.0
2,4,7,9-Tetrame...	13.614	11.5	ng	263139	3	14.730	458375	20.0
unknown15.834	15.834	11.5	ng	264373	3	14.730	458375	20.0
Pentafluoroprop...	19.213	3.0	ng	89202	4	17.480	601942	20.0
n-Tetracosanol-1	21.387	4.0	ng	126187	5	21.763	636130	20.0