LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111120\
Data File : BP003933.D
Acq On : 11 Nov 2020 22:12
Operator : CG/JU
Sample : L4631-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PAV-B11-110420-10-15.25

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

Signal : TIC: BP003933.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.928	3	7	26	rVB	7449792	9559289	100.00%	19.175%
2	3.087	26	34	44	rBV	110340	255798	2.68%	0.513%
3	3.175	44	49	63	rVB	430394	587193	6.14%	1.178%
4	5.805	489	496	507	rBV	2759797	4089848	42.78%	8.204%
5	7.452	768	776	788	rBV	2625384	4243942	44.40%	8.513%
6	8.281	910	917	923	rVB	630934	995509	10.41%	1.997%
7	9.440	1103	1114	1124	rBV	1605270	2721044	28.46%	5.458%
8	11.110	1390	1398	1405	rBV	835342	1399358	14.64%	2.807%
9	13.522	1801	1808	1823	rBV	3488843	5221963	54.63%	10.475%
10	13.728	1838	1843	1849	rBV2	71328	107119	1.12%	0.215%
11	14.322	1939	1944	1951	rVV	335693	457964	4.79%	0.919%
12	14.622	1991	1995	2001	rBV	105922	146822	1.54%	0.295%
13	14.904	2037	2043	2049	rVB	1150439	1719839	17.99%	3.450%
14	16.381	2288	2294	2315	rVB	2594724	3779336	39.54%	7.581%
15	17.634	2501	2507	2512	rBV	1365757	1935061	20.24%	3.882%
16	18.475	2646	2650	2655	rBV2	141719	221408	2.32%	0.444%
17	19.363	2793	2801	2806	rBV4	372484	670718	7.02%	1.345%
18	19.798	2872	2875	2884	rVB	276065	302472	3.16%	0.607%
19	20.098	2923	2926	2927	rBV	257527	245671	2.57%	0.493%
20	20.133	2927	2932	2938	rVB	4874230	5963077	62.38%	11.962%
21	20.763	3036	3039	3048	rVB	660961	800861	8.38%	1.606%
22	21.316	3130	3133	3142	rVB	745691	930217	9.73%	1.866%
23	21.663	3188	3192	3197	rVB2	1290138	1728328	18.08%	3.467%
24	24.145	3609	3614	3622	rVB	919930	1769023	18.51%	3.549%

Sum of corrected areas: 49851860

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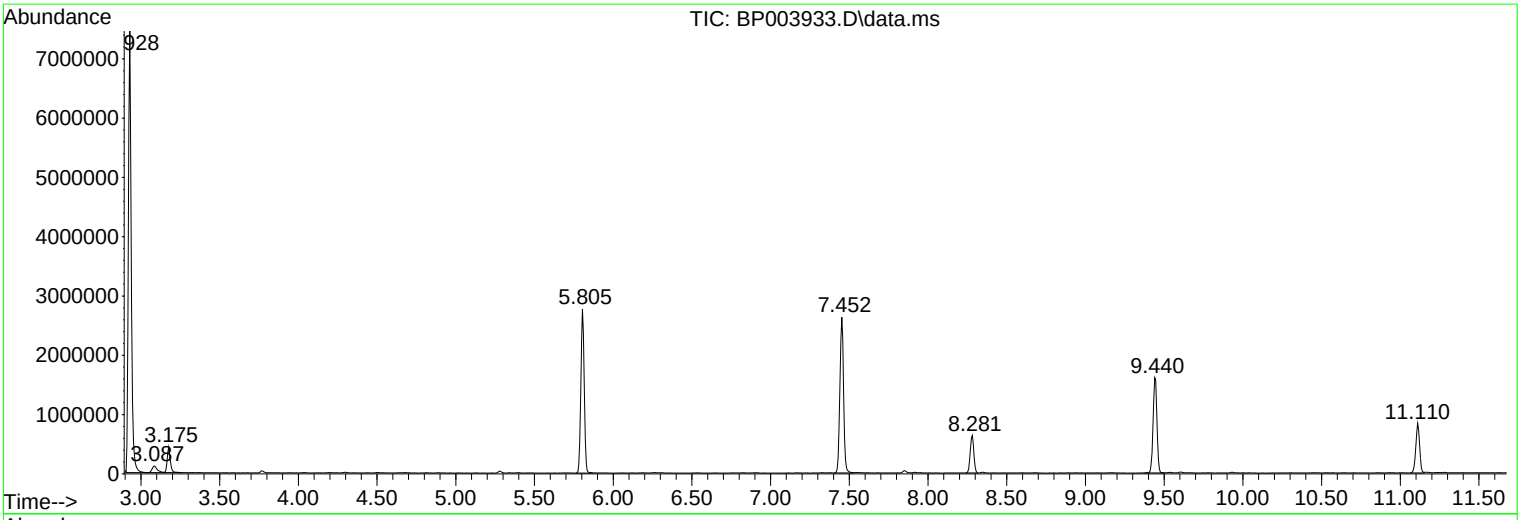
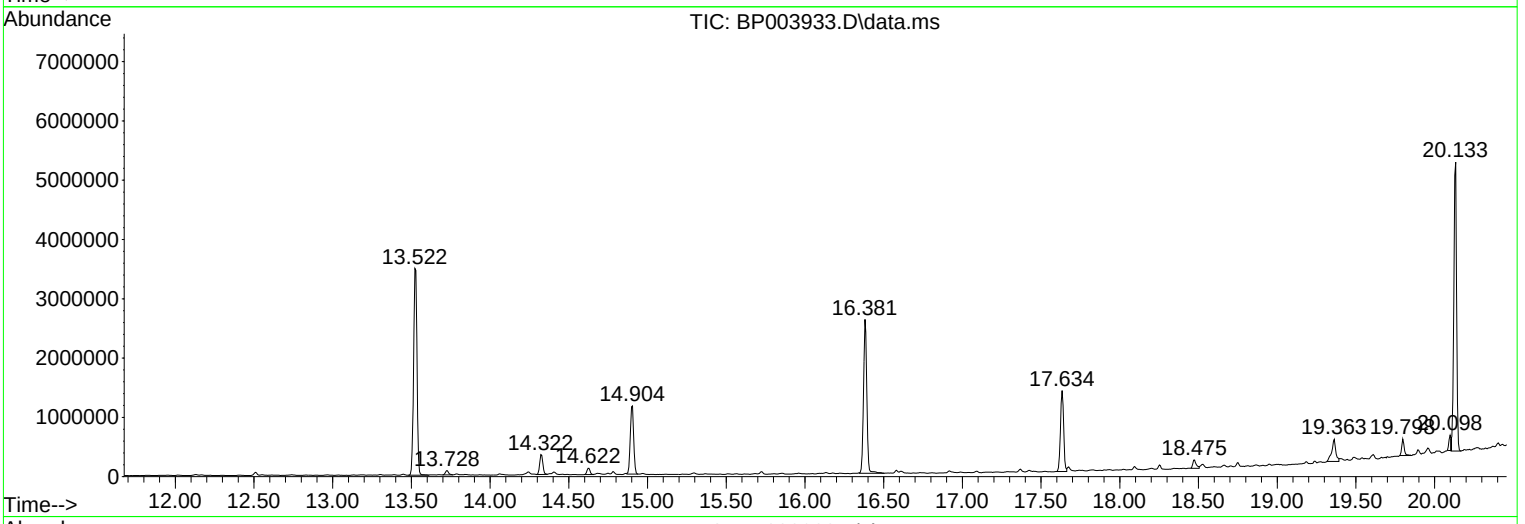
Sample : L4631-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

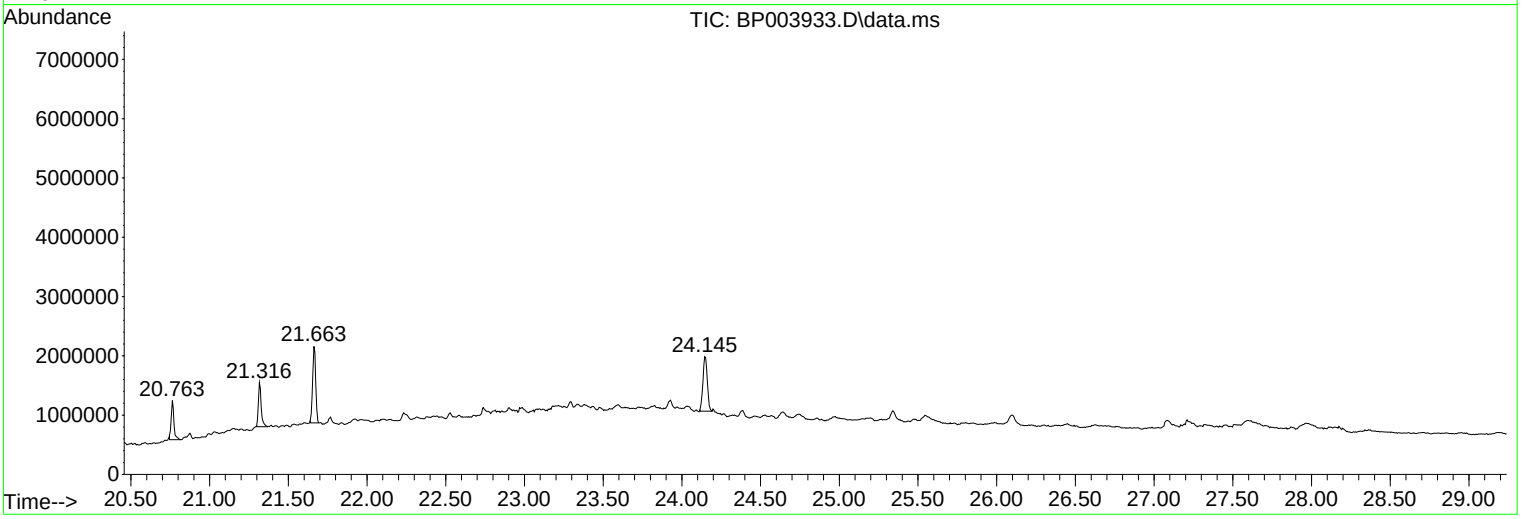
Instrument :
BNA_P
ClientSampleId :
PAV-B11-110420-10-15.25

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

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111120\
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Acq On : 11 Nov 2020 22:12
Operator : CG/JU
Sample : L4631-05
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Instrument :
BNA_P
ClientSampleId :
PAV-B11-110420-10-15.25

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

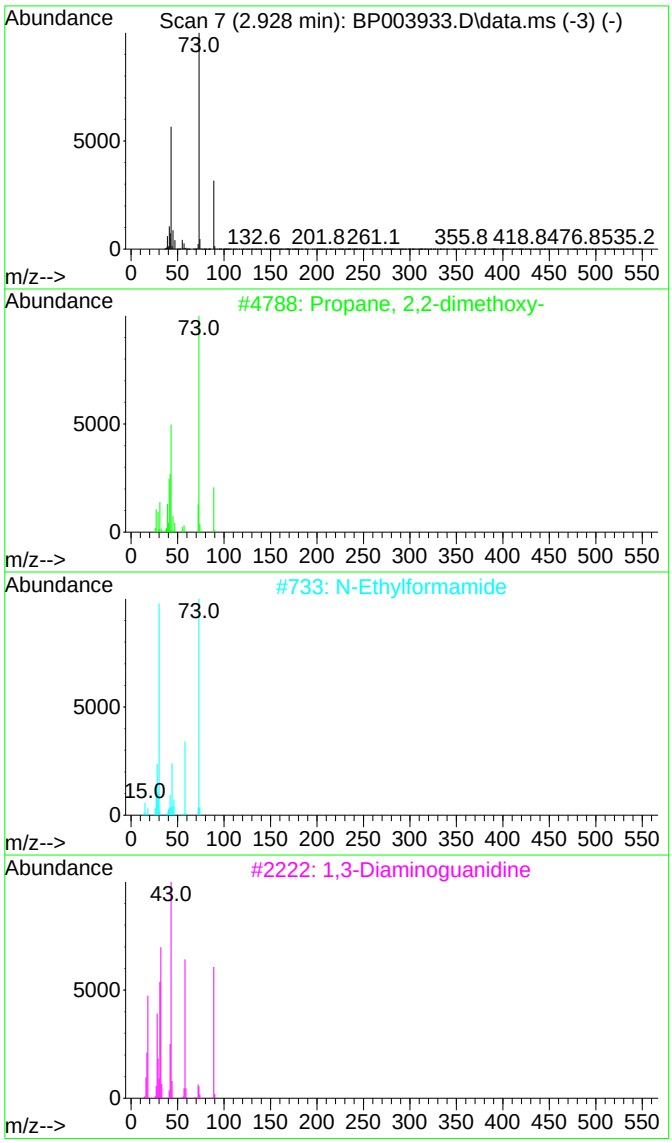
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

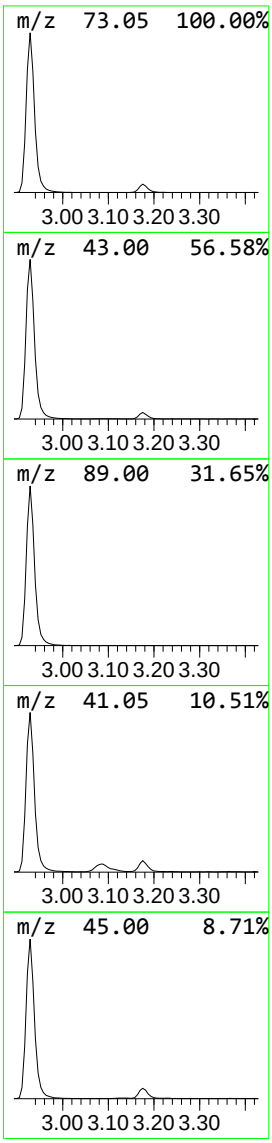
****

Peak Number 1 unknown2.928 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.928	192.05 ng	9559290	1,4-Dichlorobenzene-d4	8.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111120\
Data File : BP003933.D
Acq On : 11 Nov 2020 22:12
Operator : CG/JU
Sample : L4631-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PAV-B11-110420-10-15.25

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

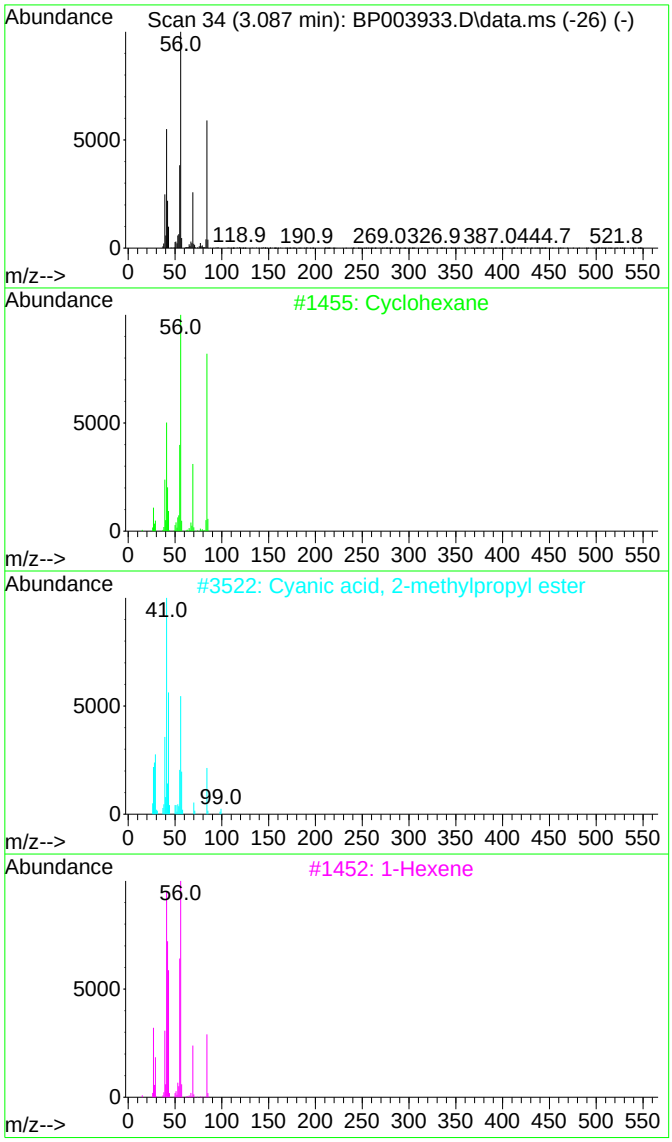
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

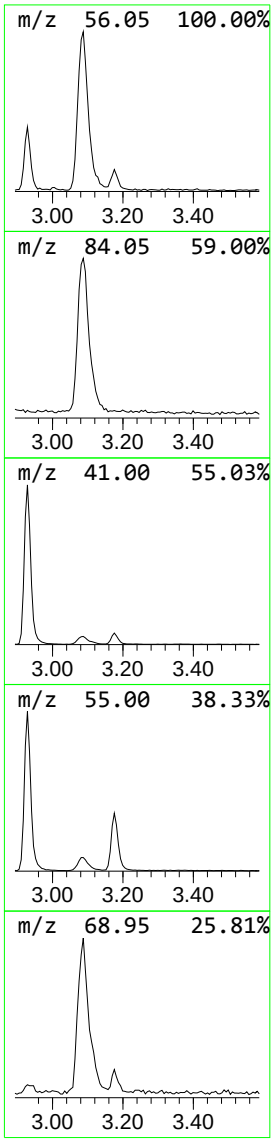
****

Peak Number 2 Cyclohexane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.087	5.14 ng	255798	1,4-Dichlorobenzene-d4	8.281

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	53
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50
5	Cyclobutane	56	C4H8	000287-23-0	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111120\
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Operator : CG/JU
Sample : L4631-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PAV-B11-110420-10-15.25

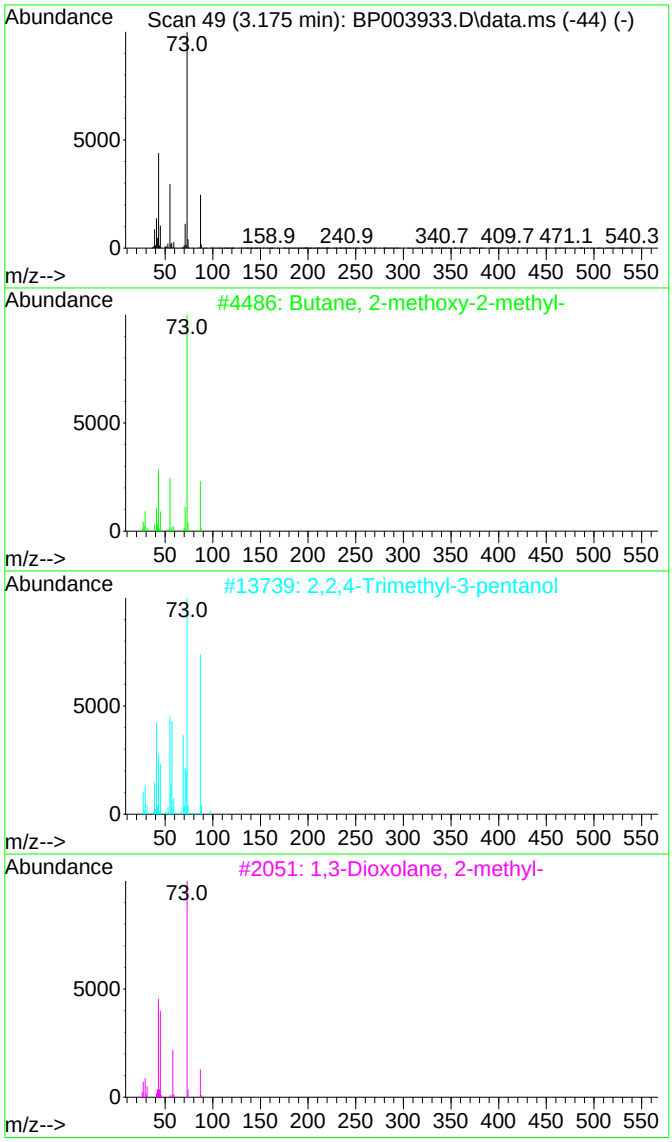
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

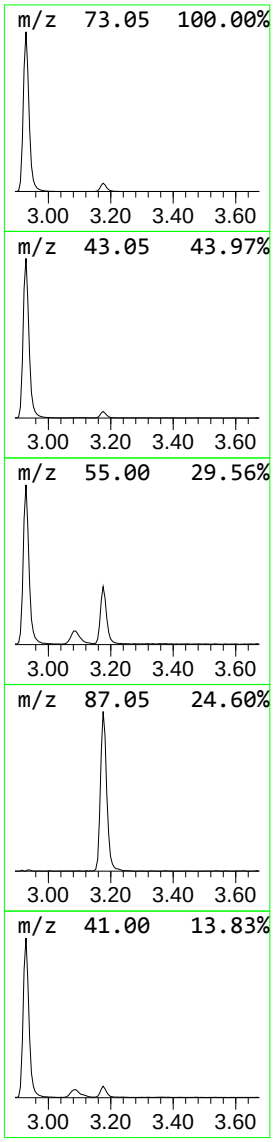
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.175	11.80 ng	587193	1,4-Dichlorobenzene-d4	8.281

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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111120\
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Sample : L4631-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PAV-B11-110420-10-15.25

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

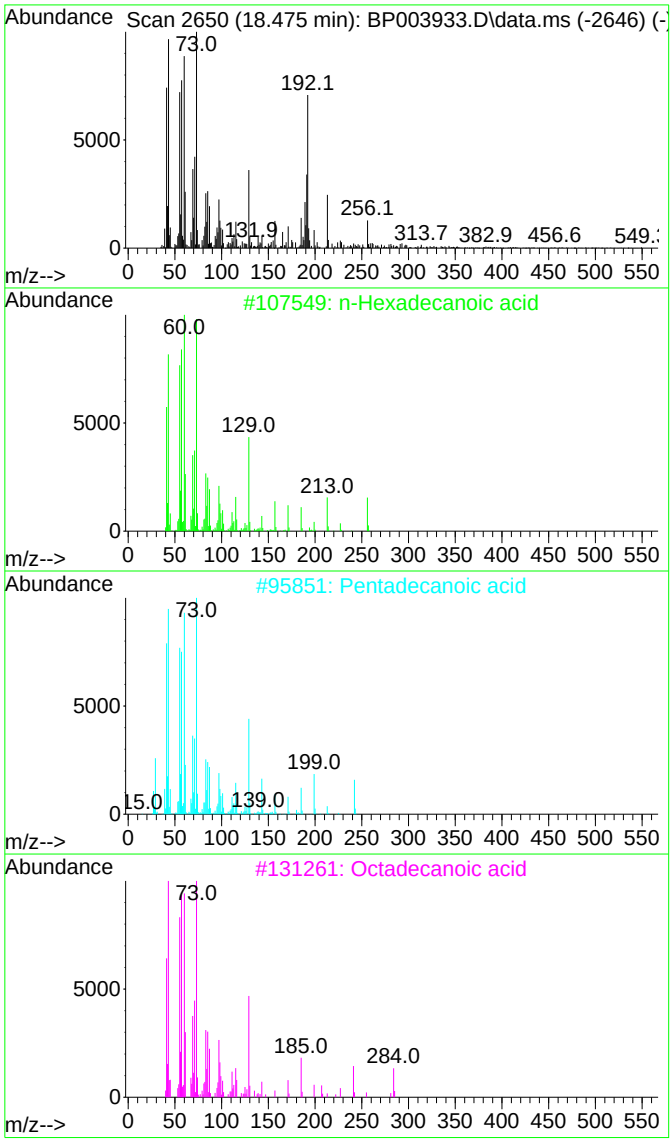
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

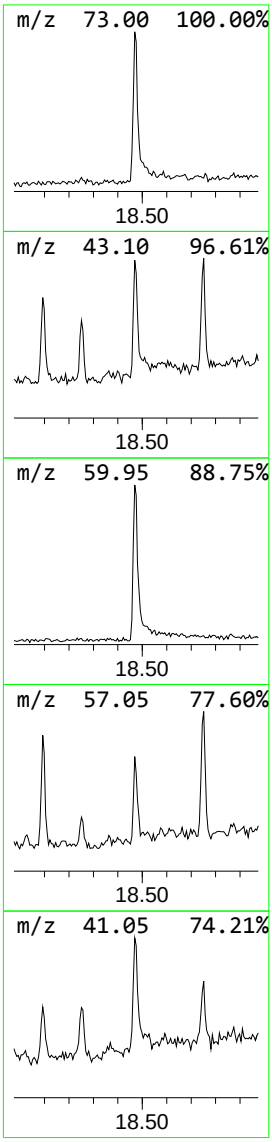
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.475	2.29 ng	221408	Phenanthrene-d10	17.634

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	83
3	Octadecanoic acid	284	C18H36O2	000057-11-4	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	78
5	Tridecanoic acid	214	C13H26O2	000638-53-9	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111120\
Data File : BP003933.D
Acq On : 11 Nov 2020 22:12
Operator : CG/JU
Sample : L4631-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : PAV-B11-110420-10-15.25

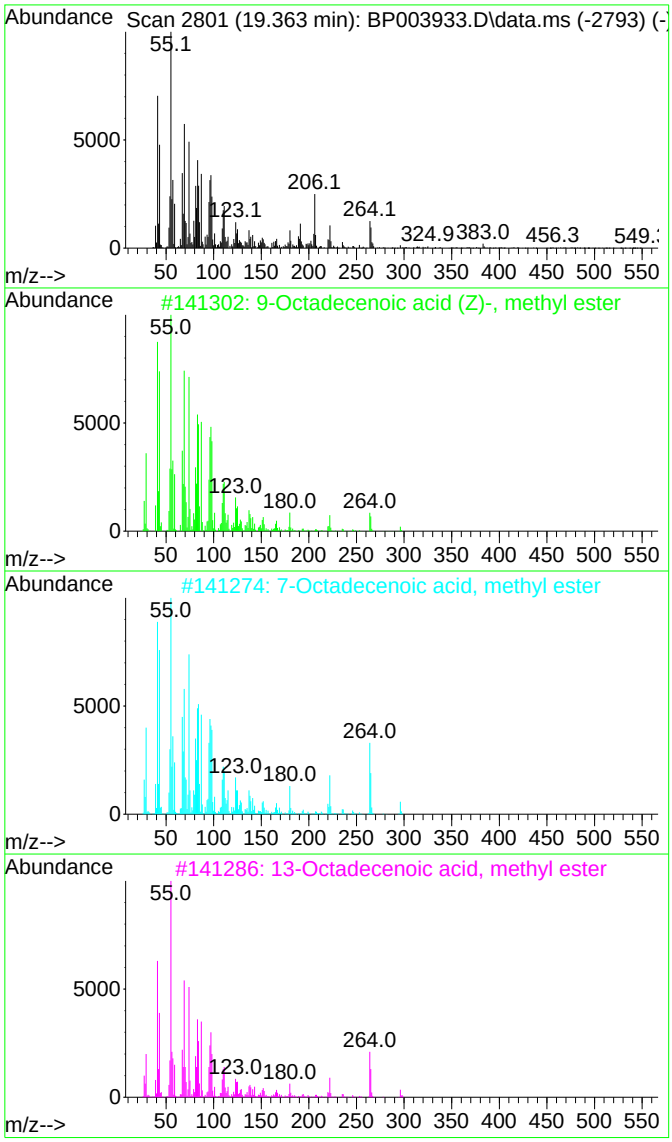
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

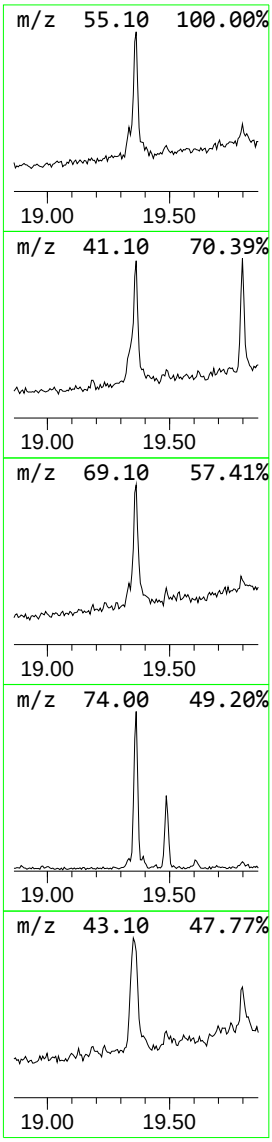
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9-Octadecenoic acid (Z)-, m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.363	6.93 ng	670718	Phenanthrene-d10	17.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	99
3	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	98
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	98
5	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	97





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Instrument :
BNA_P
ClientSampleId :
PAV-B11-110420-10-15.25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
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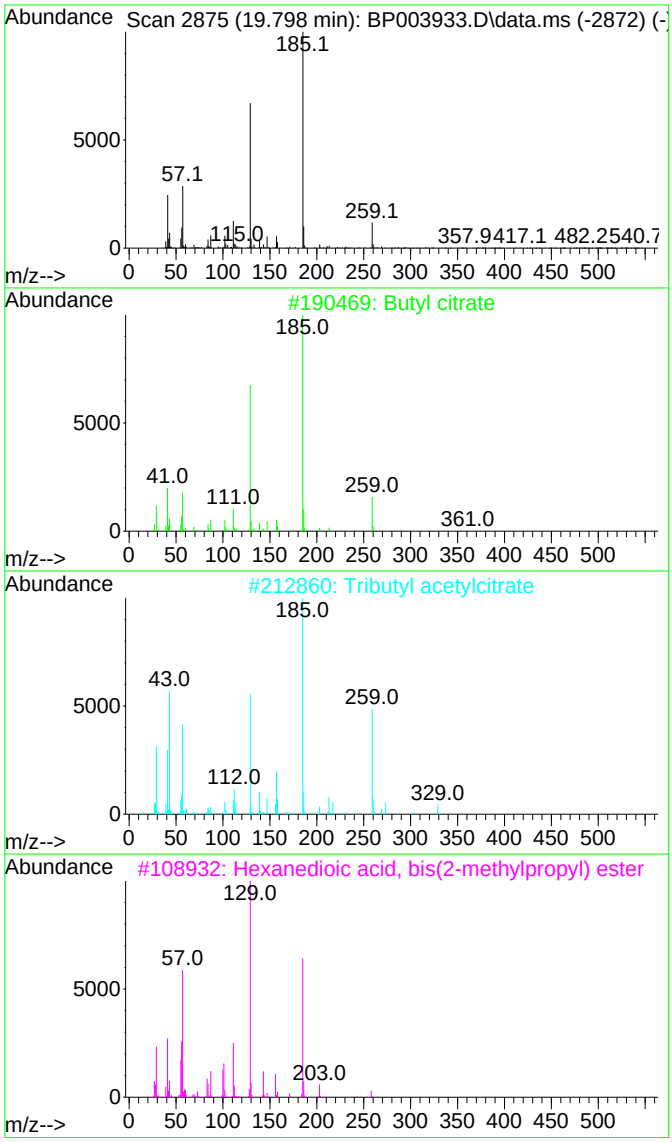
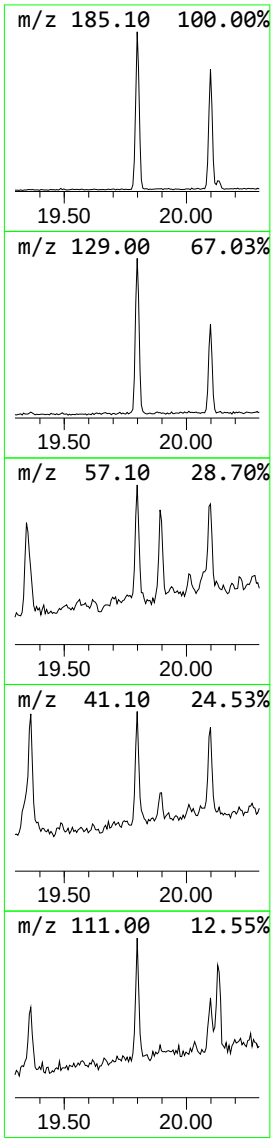
****

Peak Number 6 Butyl citrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.798	3.50 ng	302472	Chrysene-d12	21.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	91
2	Tributyl acetylcitrate	402	C20H34O8	000077-90-7	64
3	Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	56
4	Adipic acid, 2-decyl isobutyl ester	342	C20H38O4	1000353-59-6	56
5	Adipic acid, isobutyl 3-pentyl e...	272	C15H28O4	1000324-60-4	56





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Sample : L4631-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PAV-B11-110420-10-15.25

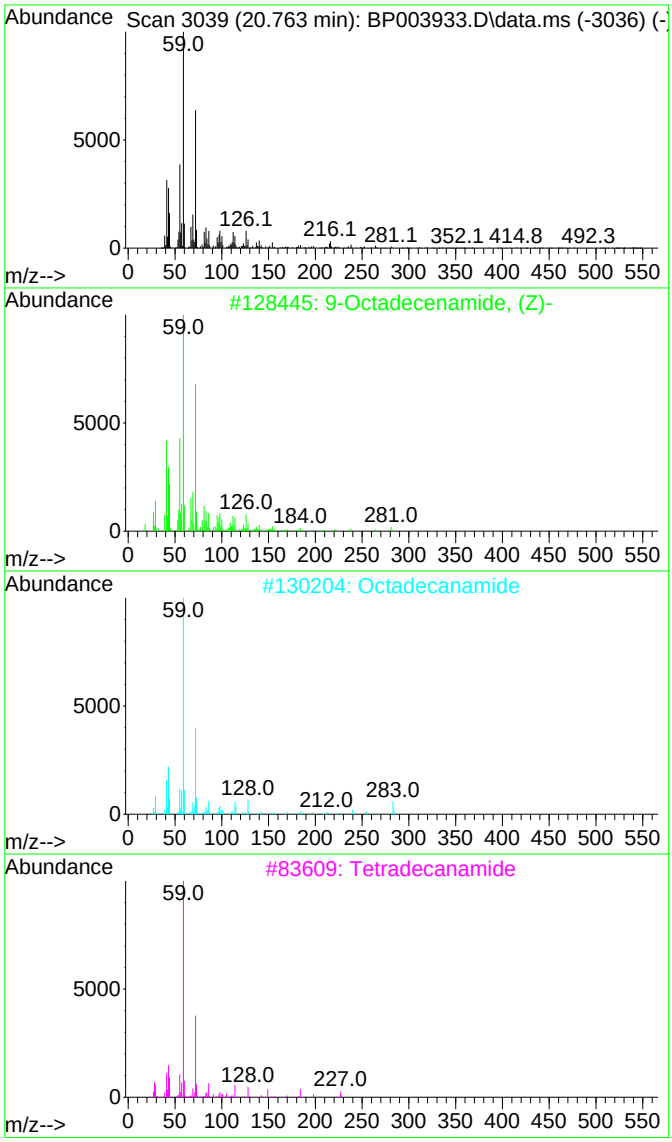
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

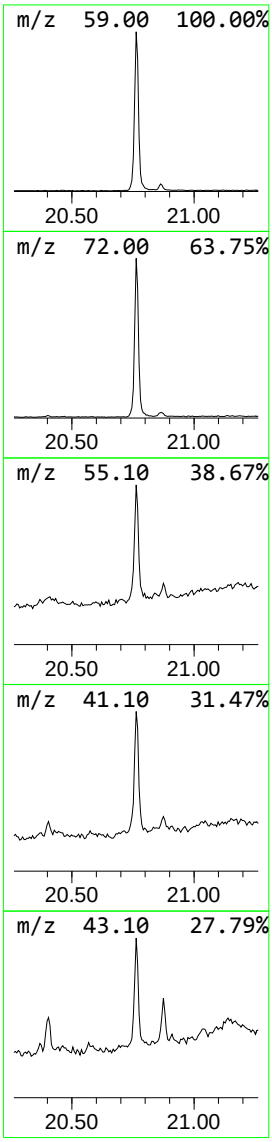
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.763	9.27 ng	800861	Chrysene-d12	21.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	89
2	Octadecanamide	283	C18H37NO	000124-26-5	78
3	Tetradecanamide	227	C14H29NO	000638-58-4	72
4	Dodecanamide	199	C12H25NO	001120-16-7	59
5	Octanamide	143	C8H17NO	000629-01-6	59





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

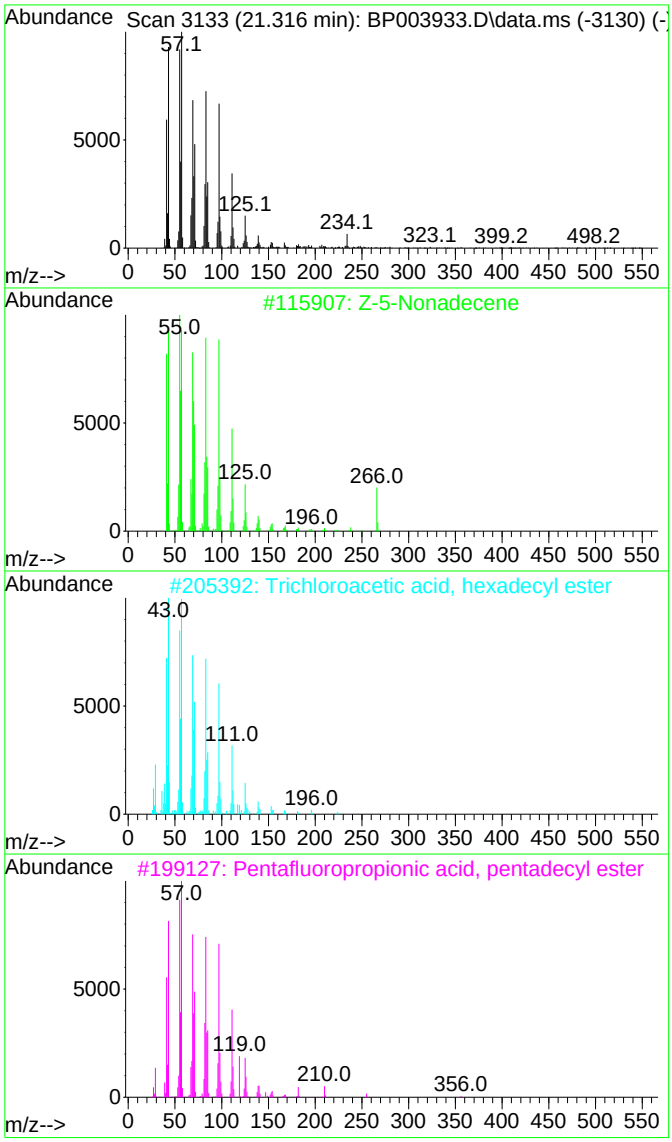
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

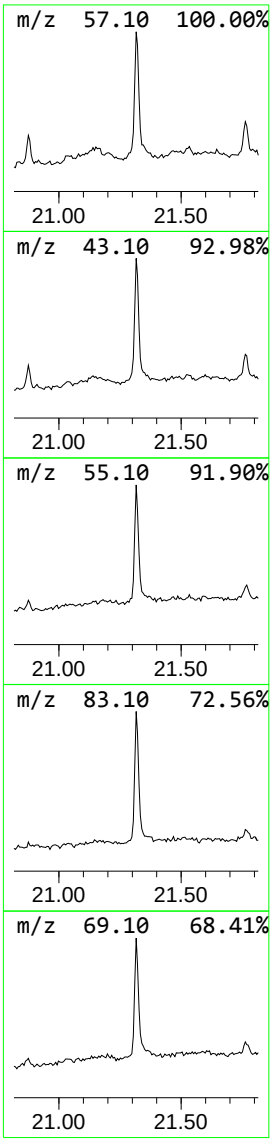
****

Peak Number 8 Z-5-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.316	10.76 ng	930217	Chrysene-d12	21.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	97
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





Tentatively Identified Compound (LSC) summary

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Data File : BP003933.D
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Instrument : BNA_P
ClientSampleId : PAV-B11-110420-10-15.25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
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
unknown2.928	2.928	192.1	ng	9559290	1	8.281	995509	20.0
Cyclohexane	3.087	5.1	ng	255798	1	8.281	995509	20.0
Butane, 2-metho...	3.175	11.8	ng	587193	1	8.281	995509	20.0
n-Hexadecanoic ...	18.475	2.3	ng	221408	4	17.634	1935060	20.0
9-Octadecenoic ...	19.363	6.9	ng	670718	4	17.634	1935060	20.0
Butyl citrate	19.798	3.5	ng	302472	5	21.663	1728330	20.0
9-Octadecenamid...	20.763	9.3	ng	800861	5	21.663	1728330	20.0
Z-5-Nonadecene	21.316	10.8	ng	930217	5	21.663	1728330	20.0