LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052821\
Data File : BF124108.D
Acq On : 28 May 2021 15:44
Operator : JU/CG
Sample : PB136683BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB136683BL

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124108.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	11	20	25	rBV2	48072	63959	2.91%	0.513%
2	5.104	509	513	522	rVB	79948	101864	4.64%	0.817%
3	5.498	575	580	583	rBV	1421830	1470357	67.00%	11.798%
4	6.504	745	751	754	rBV	1337750	1438475	65.55%	11.543%
5	6.869	809	813	817	rBB	379087	301359	13.73%	2.418%
6	7.434	903	909	912	rBV	1011628	991951	45.20%	7.960%
7	8.151	1027	1031	1035	rBV	405977	380941	17.36%	3.057%
8	9.233	1209	1215	1218	rBV	2325569	1895044	86.35%	15.206%
9	9.910	1326	1330	1334	rBV	548985	457047	20.83%	3.667%
10	10.704	1460	1465	1468	rBV	1491620	1318570	60.08%	10.580%
11	11.398	1579	1583	1587	rBV	616959	480625	21.90%	3.857%
12	12.992	1849	1854	1857	rBV	2482472	2194538	100.00%	17.609%
13	13.839	1990	1998	2000	rBV	47308	62260	2.84%	0.500%
14	13.874	2000	2004	2006	rVV	63676	71895	3.28%	0.577%
15	13.910	2006	2010	2015	rVB	170453	163366	7.44%	1.311%
16	14.045	2026	2033	2036	rBV	459047	423901	19.32%	3.401%
17	14.510	2107	2112	2115	rBV	37506	35447	1.62%	0.284%
18	14.821	2159	2165	2169	rVB	46671	50735	2.31%	0.407%
19	15.168	2218	2224	2229	rBV	54832	68065	3.10%	0.546%
20	15.527	2280	2285	2289	rBV	272130	360043	16.41%	2.889%
21	15.557	2289	2290	2295	rVB	44769	39612	1.81%	0.318%
22	16.004	2362	2366	2371	rVB3	32887	50805	2.32%	0.408%
23	16.521	2447	2454	2458	rBV2	21882	41483	1.89%	0.333%

Sum of corrected areas: 12462342

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Misc :
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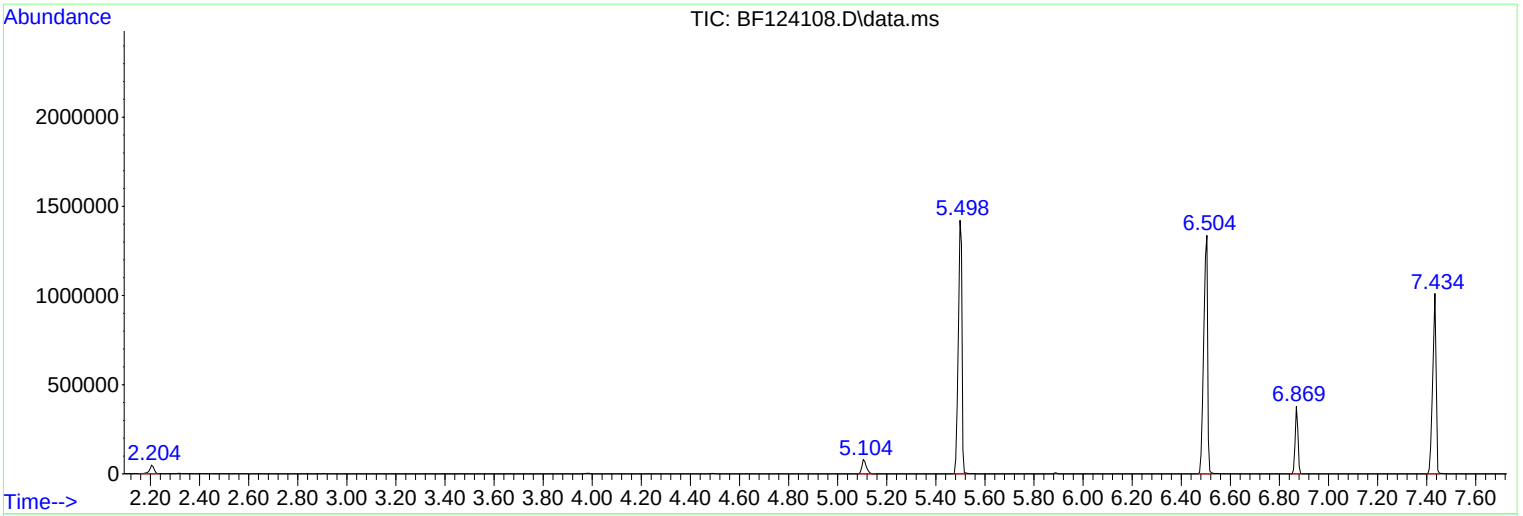
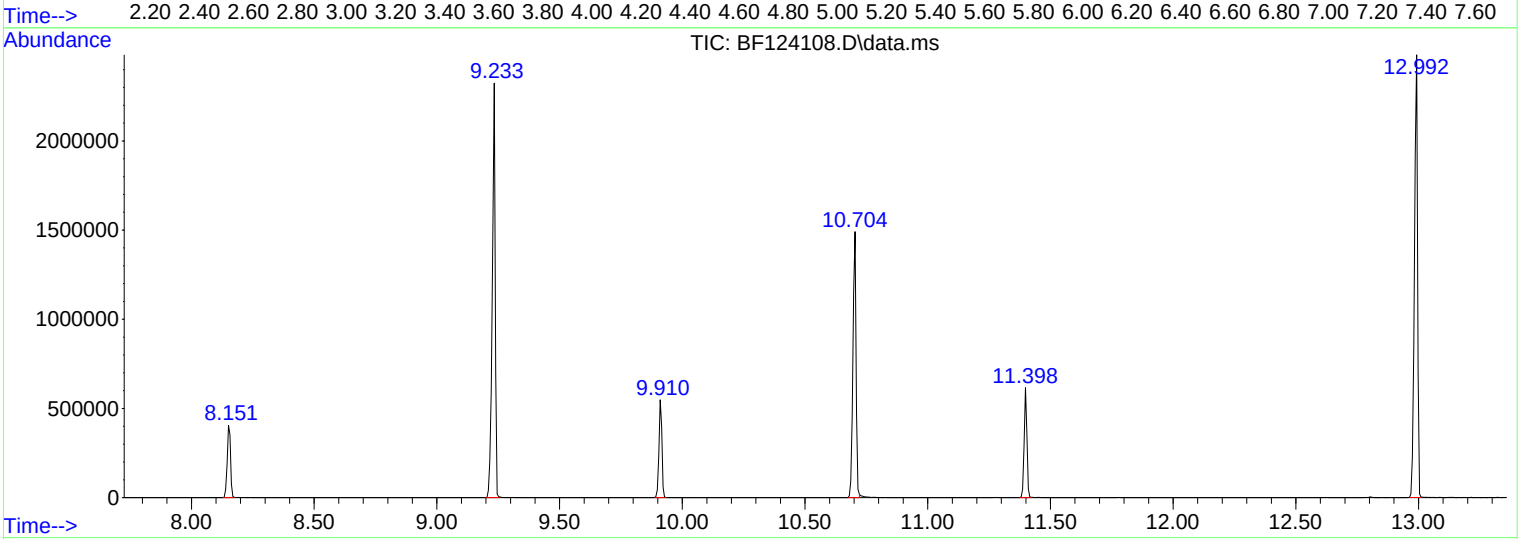
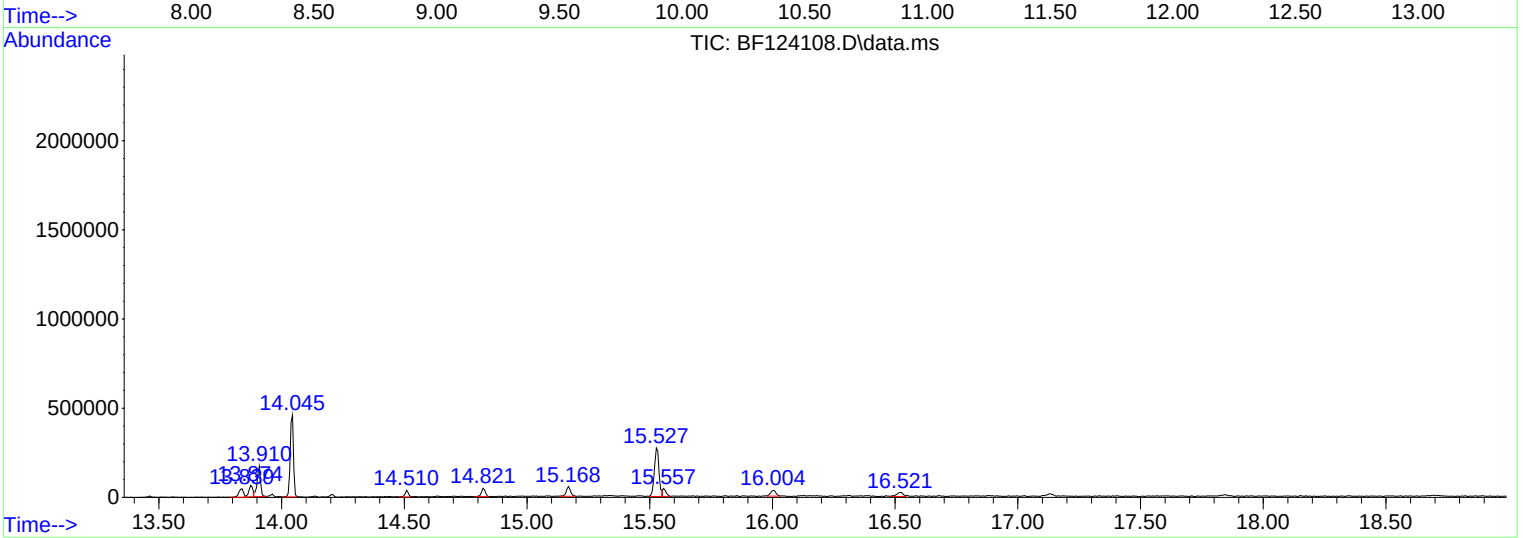
Instrument :
BNA_F
ClientSampleId :
PB136683BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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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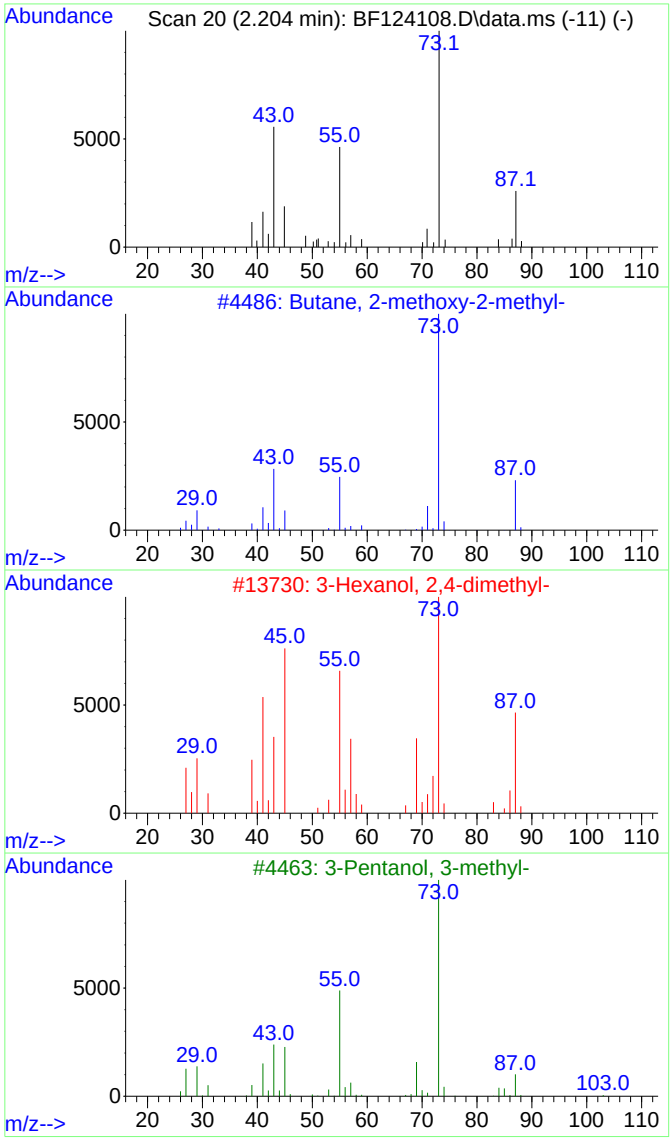
TIC Integration Parameters: LSCINT.P

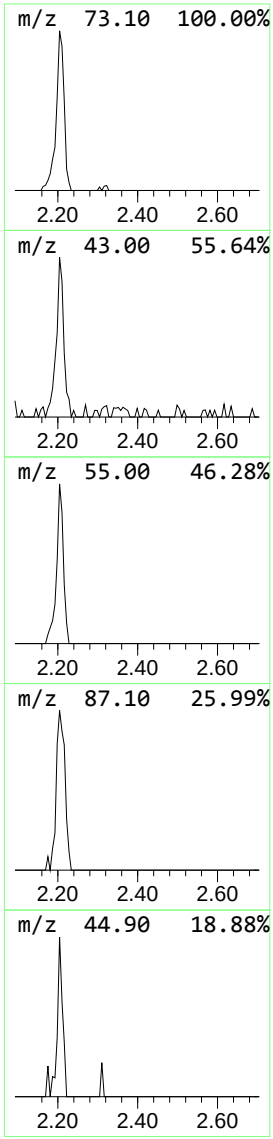
****

Peak Number 1 unknown2.20 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	4.24 ng	63959	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	45
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	42
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4	1-Pentanamine	87	C5H13N	000110-58-7	17
5	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12





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Operator : JU/CG
Sample : PB136683BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB136683BL

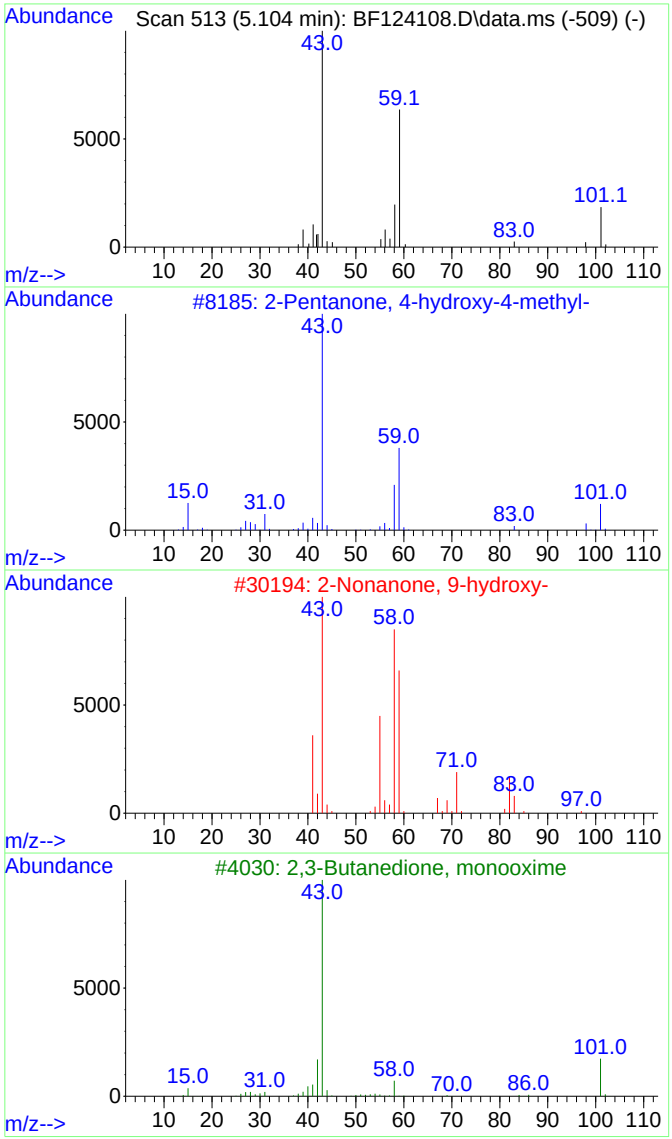
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

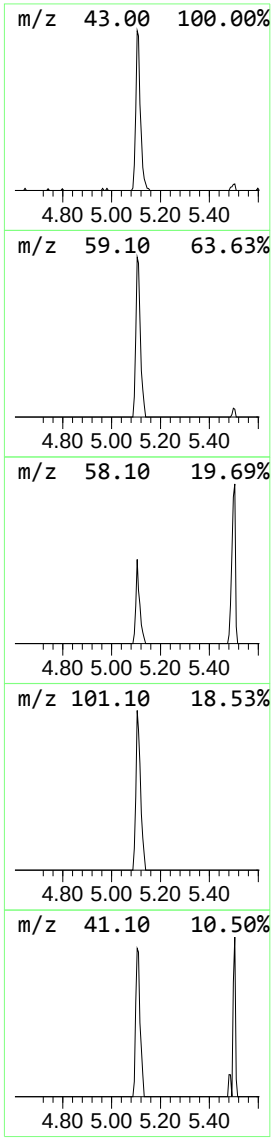
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	6.76 ng	101864	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4	Acetone	58	C3H6O	000067-64-1	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





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Sample : PB136683BL
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ALS Vial : 3 Sample Multiplier: 1

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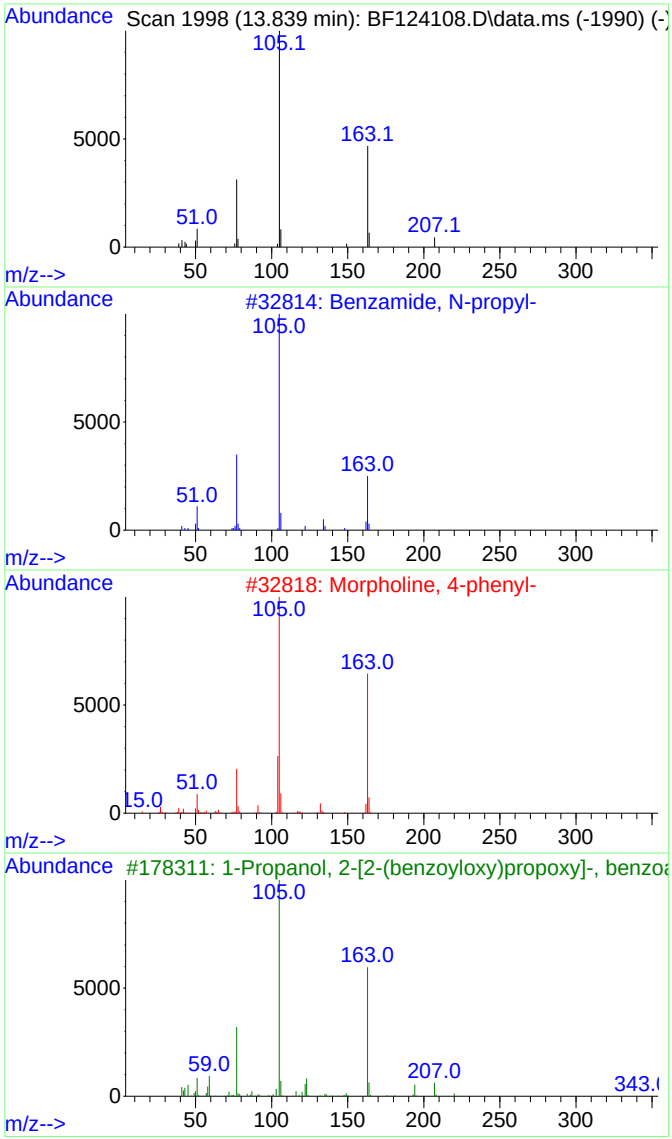
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

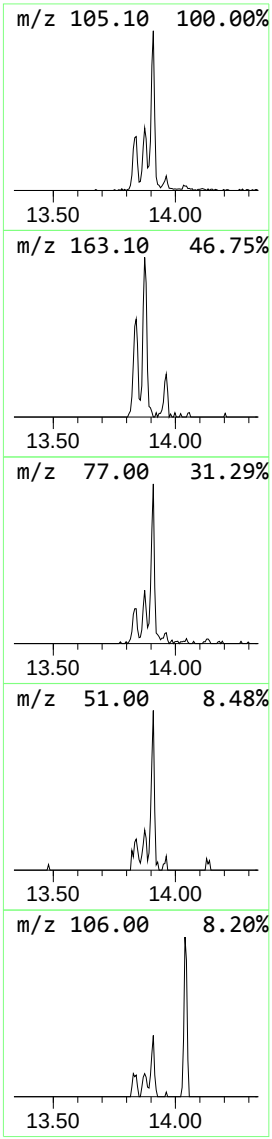
****

Peak Number 3 Benzamide, N-propyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	2.94 ng	62260	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	86
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
3	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	64
4	Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	56
5	Ethanone, 2-(formyloxy)-1-phenyl-	164	C9H8O3	055153-12-3	38





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ClientSampleId :
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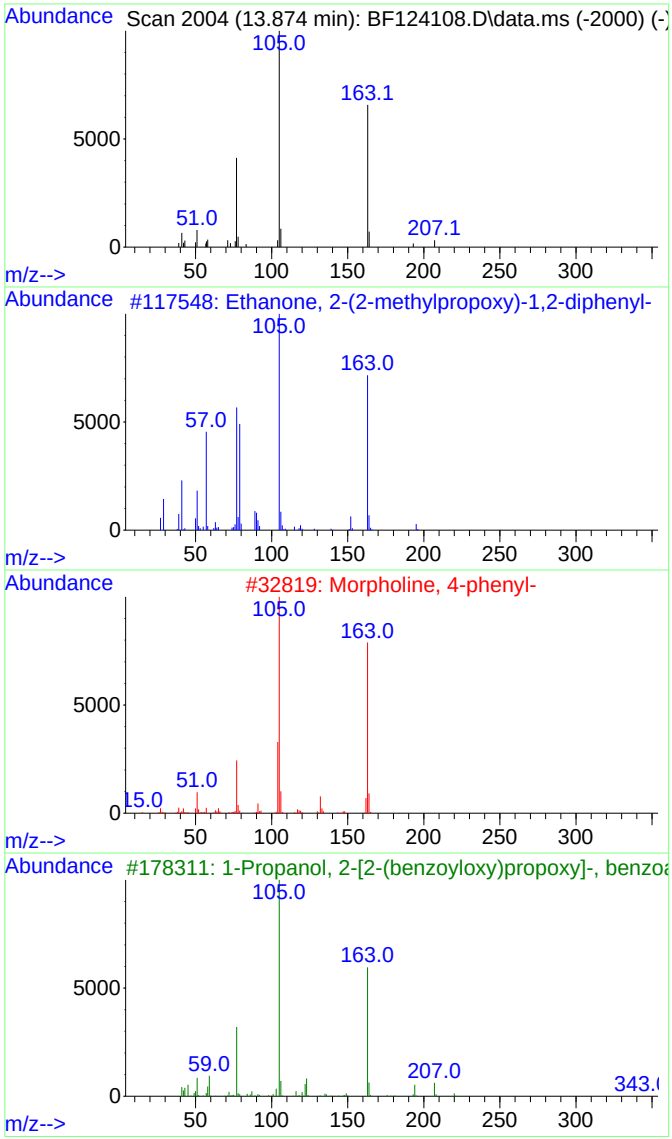
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

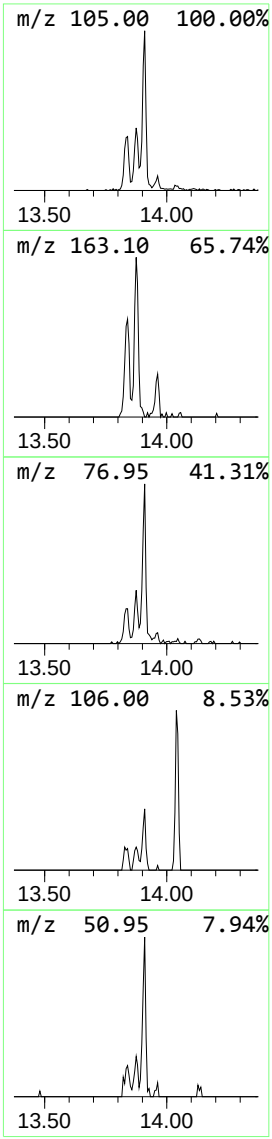
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanone, 2-(2-methylpropox... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.39 ng	71895	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 2-(2-methylpropoxy)-1,...	268	C18H20O2	022499-12-3	78
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	59
3	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	56
4	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	53
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	43





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Sample : PB136683BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

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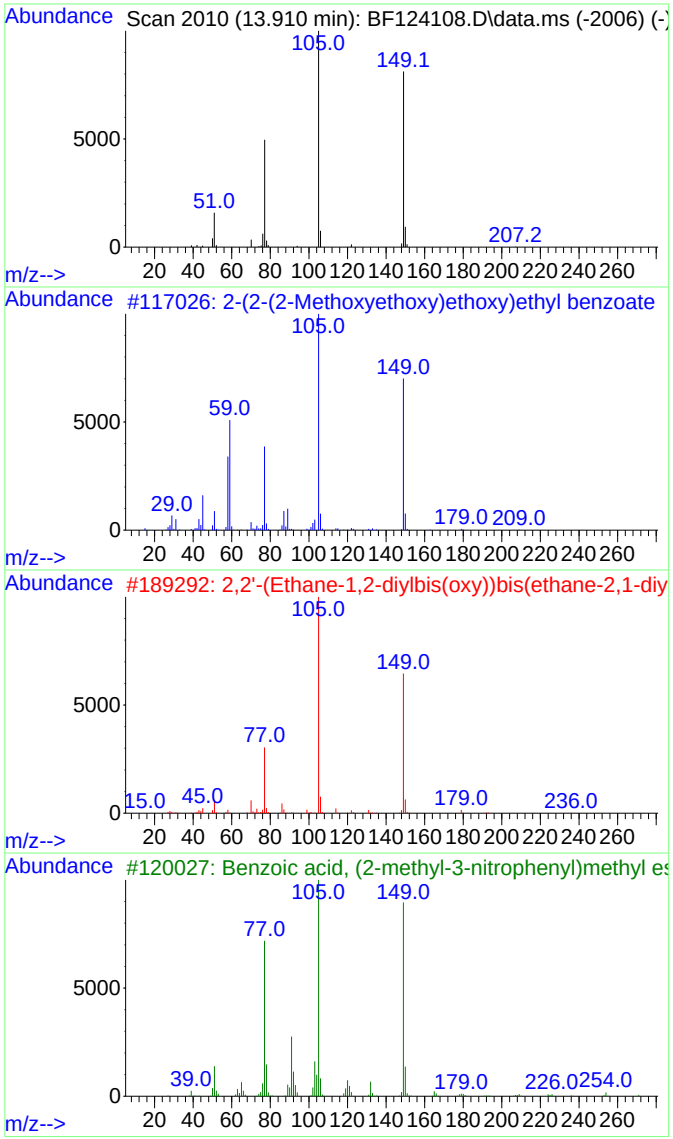
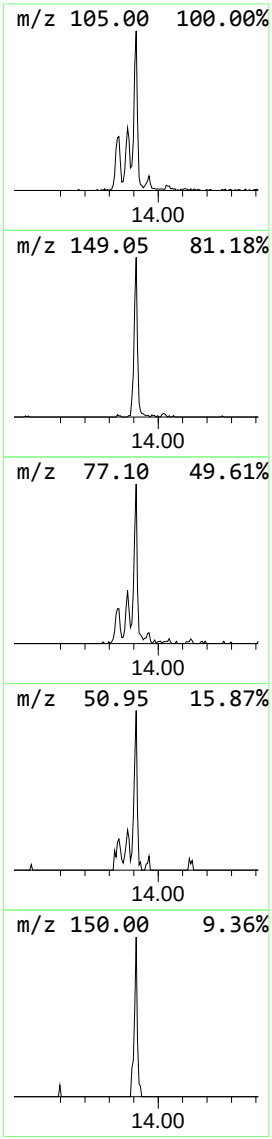
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-(2-(2-Methoxyethoxy)ethox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	7.71 ng	163366	Chrysene-d12	14.045

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	83
2	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	74
3	Benzoic acid, (2-methyl-3-nitrop...	271	C15H13NO4	1000367-95-0	74
4	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	74
5	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	47





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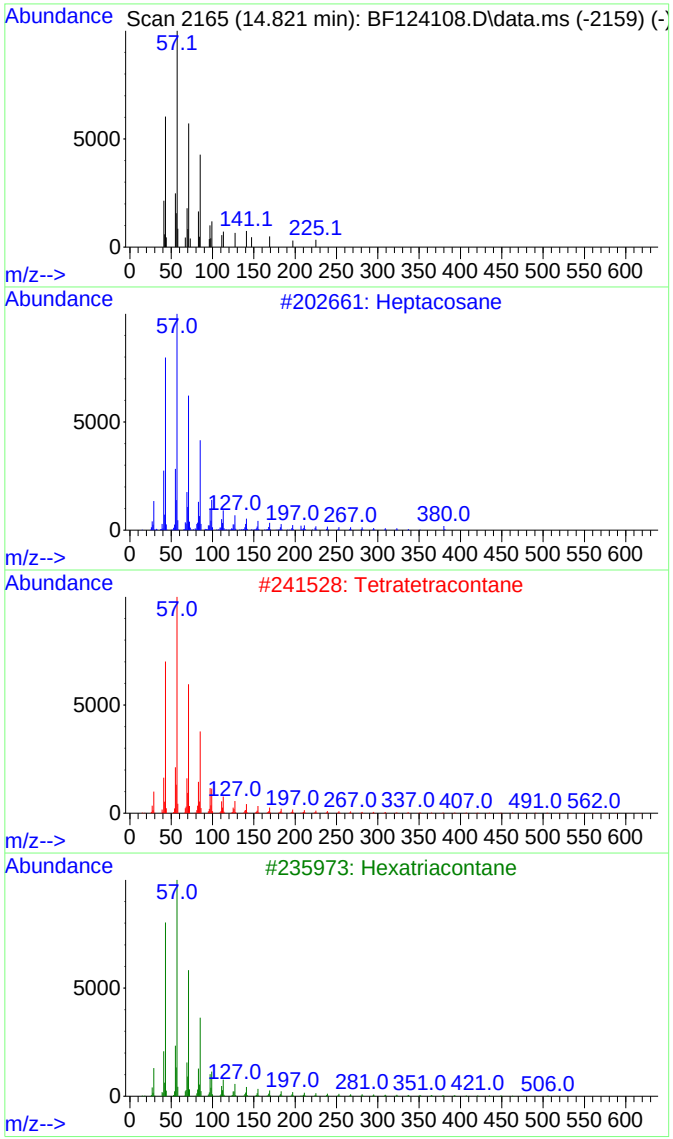
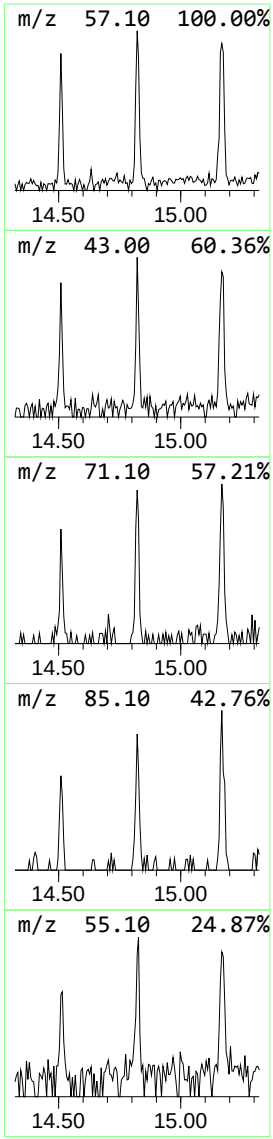
****

Peak Number 6 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	2.82 ng	50735	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Hexatriacontane	507	C36H74	000630-06-8	86
4	2-methyloctacosane	408	C29H60	1000376-72-8	86
5	Octacosane	394	C28H58	000630-02-4	86





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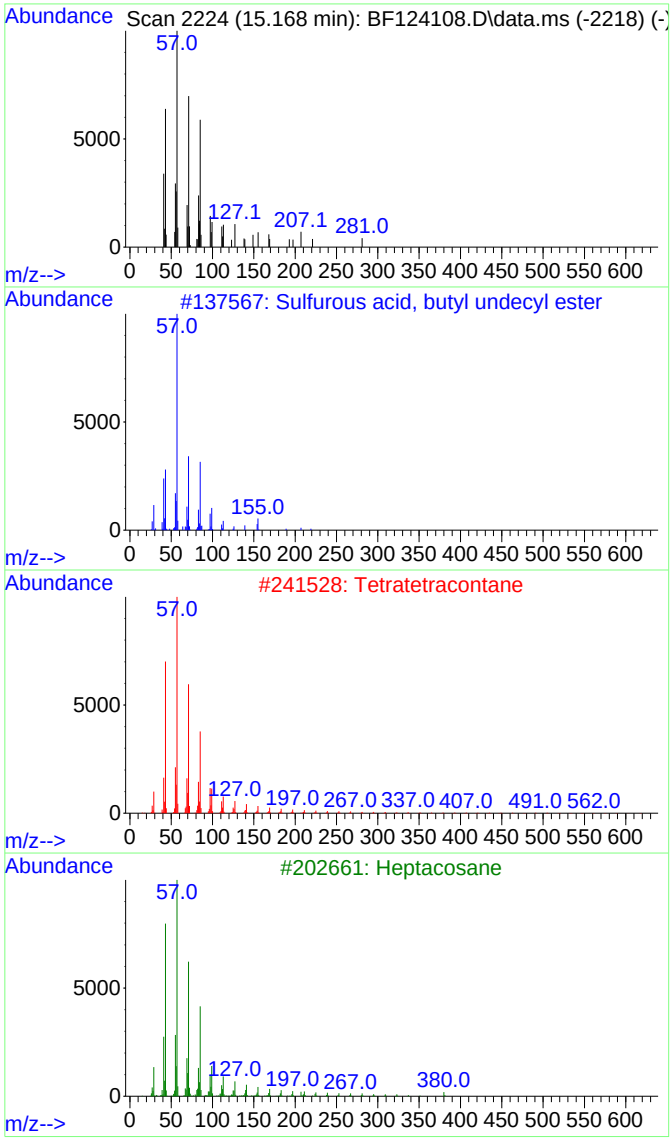
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

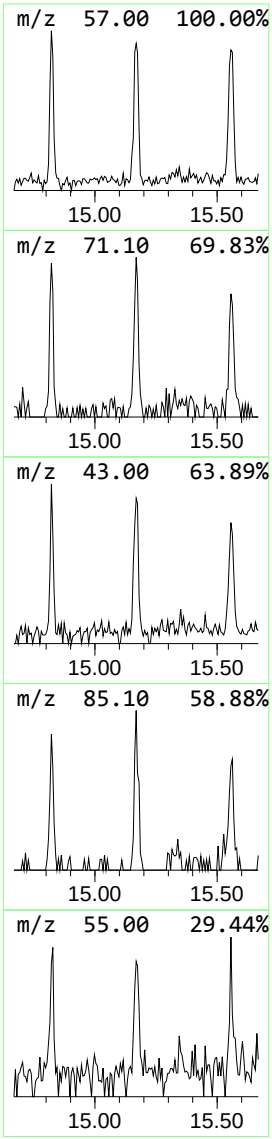
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Sulfurous acid, butyl undec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.168	3.78 ng	68065	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	59
2	Tetratetracontane	619	C44H90	007098-22-8	58
3	Heptacosane	380	C27H56	000593-49-7	58
4	Hentriacontane	437	C31H64	000630-04-6	53
5	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	53





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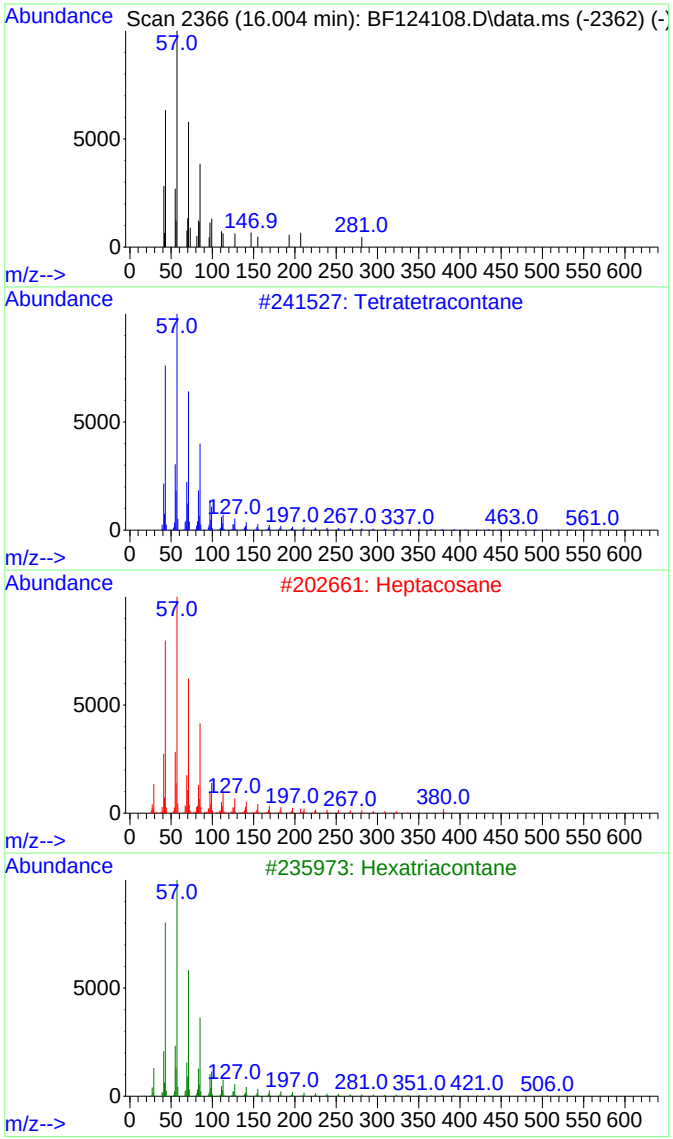
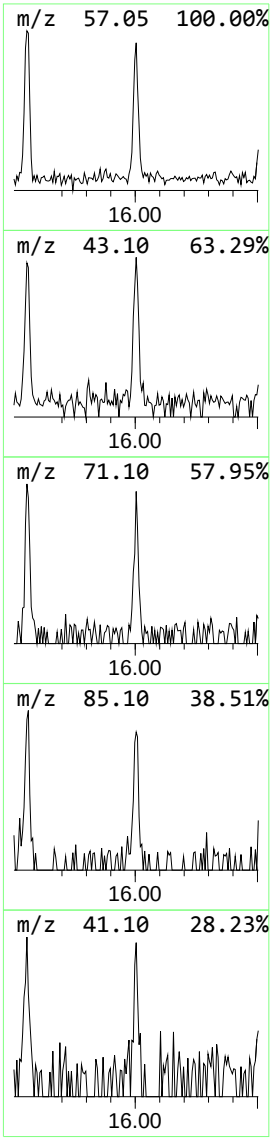
****

Peak Number 8 Tetratetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.004	2.82 ng	50805	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	72
2	Heptacosane	380	C27H56	000593-49-7	72
3	Hexatriacontane	507	C36H74	000630-06-8	72
4	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	64
5	Heptadecane	240	C17H36	000629-78-7	64





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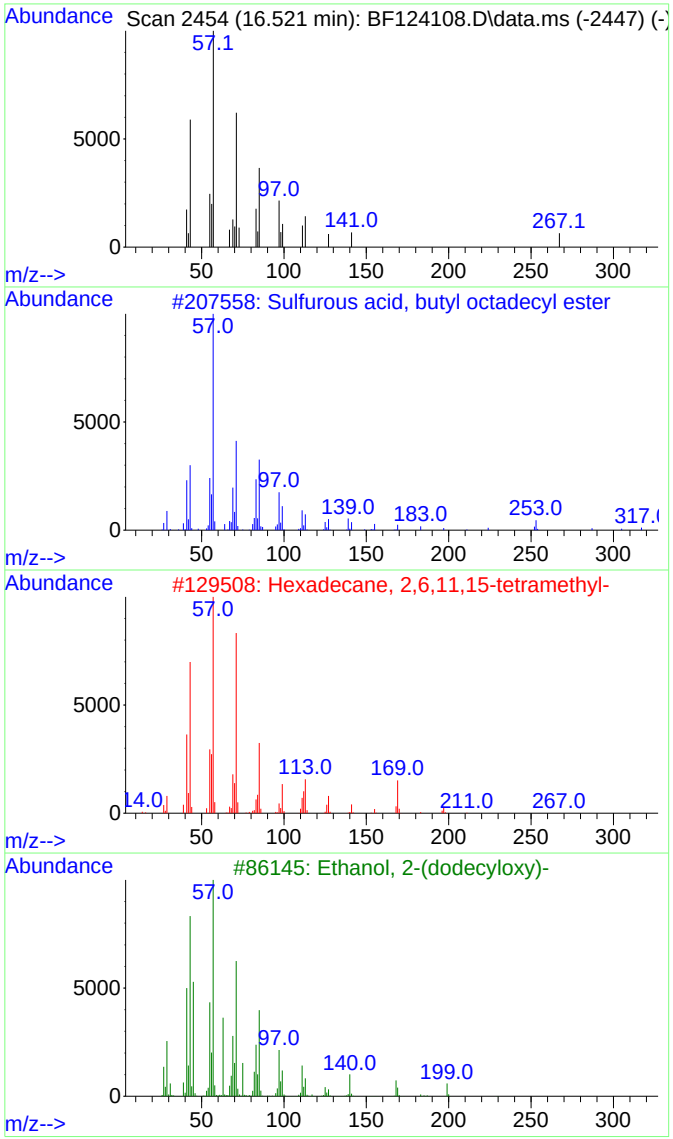
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

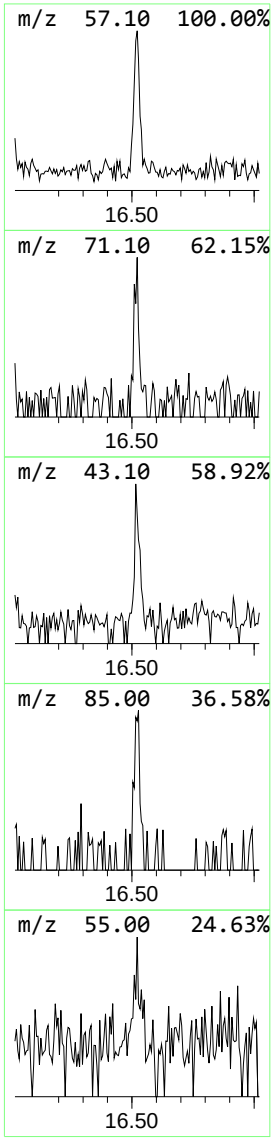
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Sulfurous acid, butyl octad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.521	2.30 ng	41483	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	78
2	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	72
3	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	72
4	Tetratetracontane	619	C44H90	007098-22-8	72
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
ClientSampleId : PB136683BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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
unknown2.20	2.204	4.2	ng	63959	1	6.869	301359	20.0
2-Pentanone, 4-...	5.104	6.8	ng	101864	1	6.869	301359	20.0
Benzamide, N-pr...	13.839	2.9	ng	62260	5	14.045	423901	20.0
Ethanone, 2-(2-...	13.874	3.4	ng	71895	5	14.045	423901	20.0
2-(2-(2-Methoxy...	13.910	7.7	ng	163366	5	14.045	423901	20.0
Heptacosane	14.821	2.8	ng	50735	6	15.527	360043	20.0
Sulfurous acid,...	15.168	3.8	ng	68065	6	15.527	360043	20.0
Tetratetracontane	16.004	2.8	ng	50805	6	15.527	360043	20.0
Sulfurous acid,...	16.521	2.3	ng	41483	6	15.527	360043	20.0