LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042224\
Data File : BG060994.D
Acq On : 22 Apr 2024 16:43
Operator : MA/JU
Sample : P2147-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COMP-B

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-BG042024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060994.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	% max.	% of total
1	3.169	25	31	41	rVB2	24317	47611	2.78%	0.564%
2	3.686	114	119	125	rBV	26166	41699	2.44%	0.494%
3	5.531	426	433	443	rVB	360688	570261	33.35%	6.756%
4	7.111	695	702	714	rVB	376476	626677	36.64%	7.425%
5	7.940	836	843	850	rBV2	107473	175300	10.25%	2.077%
6	9.091	1031	1039	1047	rBV	247335	428407	25.05%	5.076%
7	10.507	1272	1280	1288	rBV3	10024	17597	1.03%	0.208%
8	10.736	1312	1319	1325	rBV	129310	228366	13.35%	2.706%
9	13.192	1730	1737	1744	rBV	664915	990503	57.92%	11.735%
10	14.215	1902	1911	1919	rBV2	17219	24320	1.42%	0.288%
11	14.514	1952	1962	1966	rBV2	192905	305773	17.88%	3.623%
12	14.567	1966	1971	1979	rVB	225387	347956	20.35%	4.122%
13	14.773	2000	2006	2007	rBV3	16911	22001	1.29%	0.261%
14	14.791	2007	2009	2015	rVB2	18279	22554	1.32%	0.267%
15	16.060	2218	2225	2232	rBV	574529	887641	51.90%	10.516%
16	16.336	2267	2272	2282	rBV2	69105	108776	6.36%	1.289%
17	17.317	2431	2439	2443	rBV	294489	429492	25.11%	5.088%
18	17.358	2443	2446	2450	rVB	26190	35383	2.07%	0.419%
19	17.875	2529	2534	2537	rBV	13193	17496	1.02%	0.207%
20	18.216	2583	2592	2600	rBV5	32948	71807	4.20%	0.851%
21	19.368	2783	2788	2793	rBV	87887	119002	6.96%	1.410%
22	19.732	2845	2850	2856	rVB	71971	110546	6.46%	1.310%
23	19.937	2879	2885	2895	rVB	1325353	1710154	100.00%	20.261%
24	20.225	2931	2934	2937	rBV5	16395	17912	1.05%	0.212%
25	21.248	3104	3108	3113	rBV5	52061	83658	4.89%	0.991%
26	21.571	3156	3163	3169	rBV2	292932	540123	31.58%	6.399%
27	24.697	3688	3695	3706	rBV	175047	459640	26.88%	5.446%

Sum of corrected areas: 8440655

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Instrument :
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ClientSampleId :
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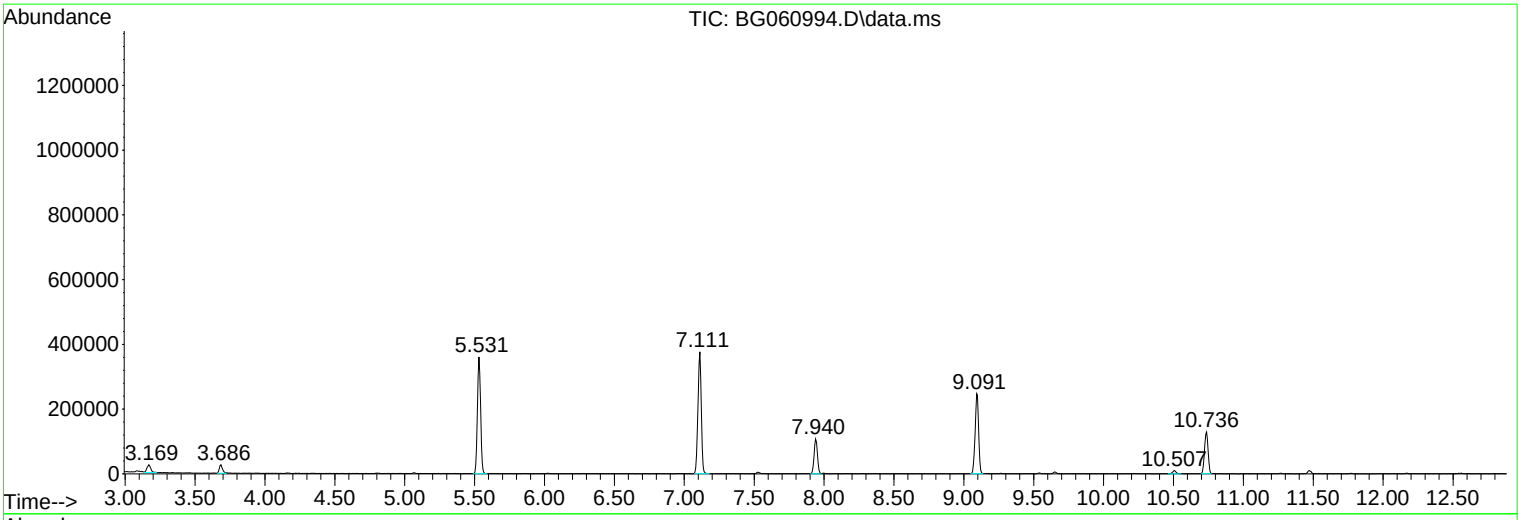
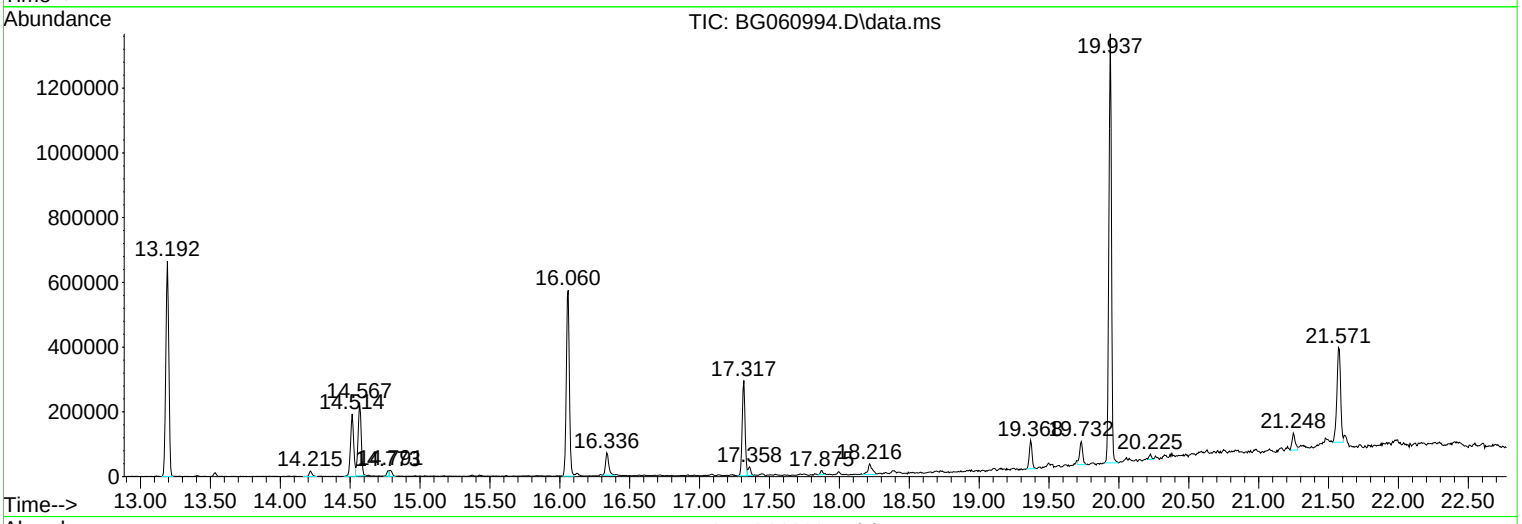
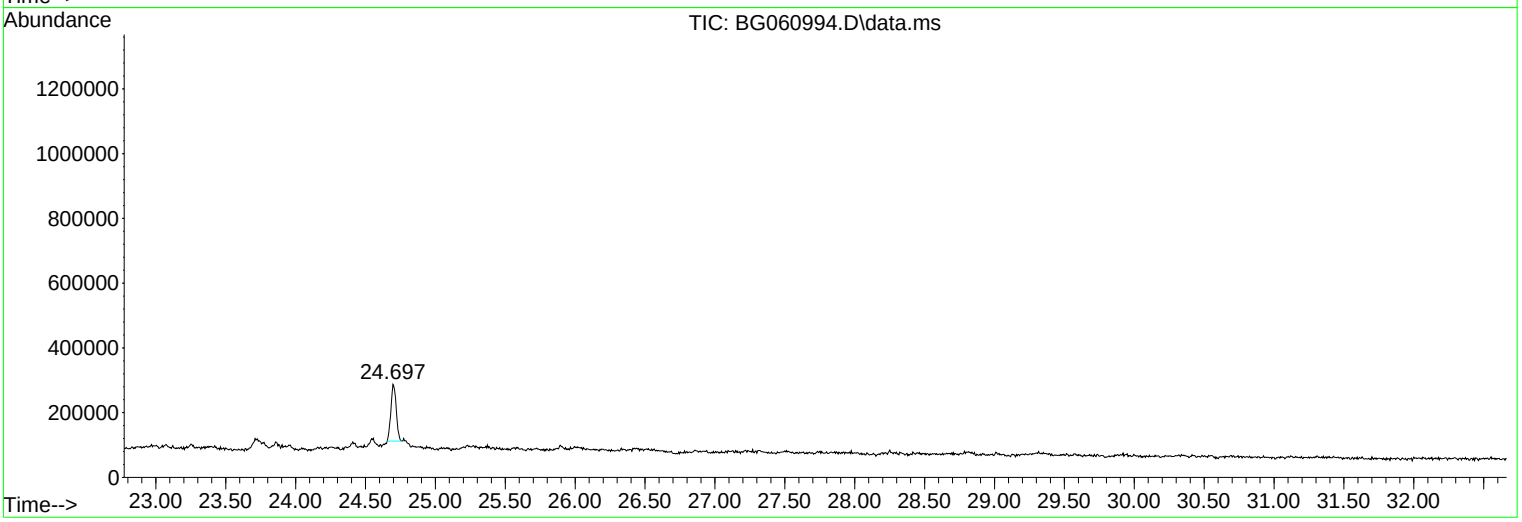
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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TIC Library : C:\Database\NIST20.L
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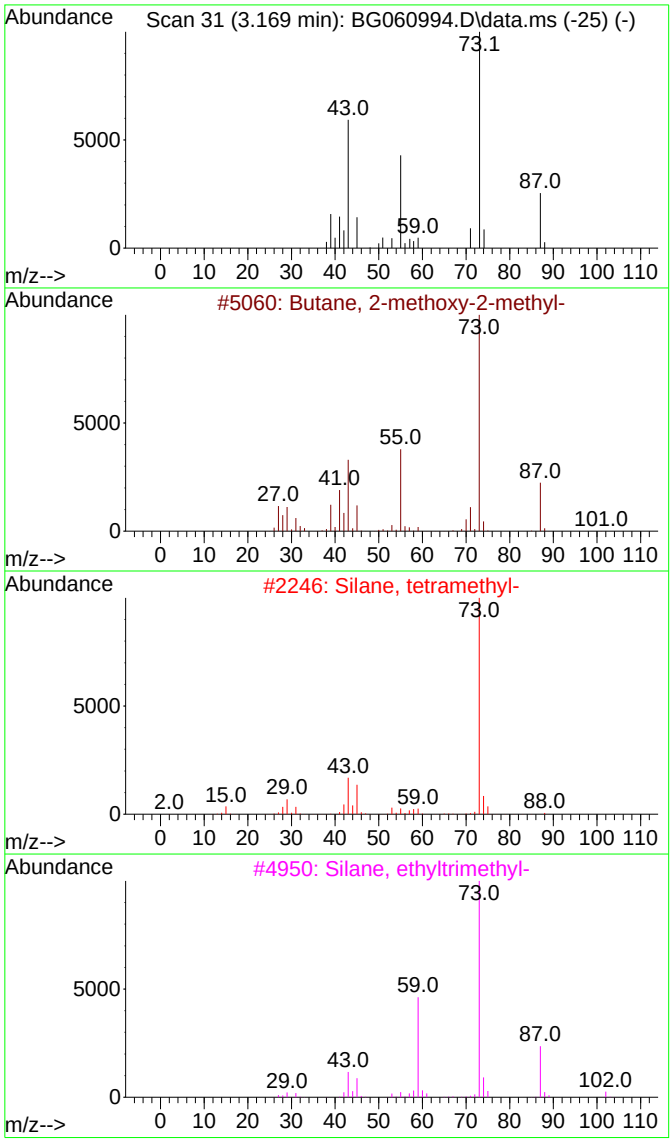
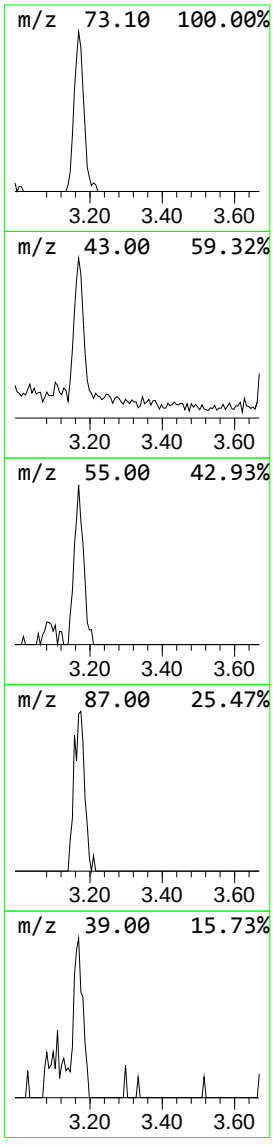
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.169	5.43 ng	47611	1,4-Dichlorobenzene-d4	7.940

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4	1-Propene-1-thiol	74	C3H6S	000925-89-3	35
5	(3S)-3-Pyrrolidinol	87	C4H9NO	100243-39-8	14





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Sample : P2147-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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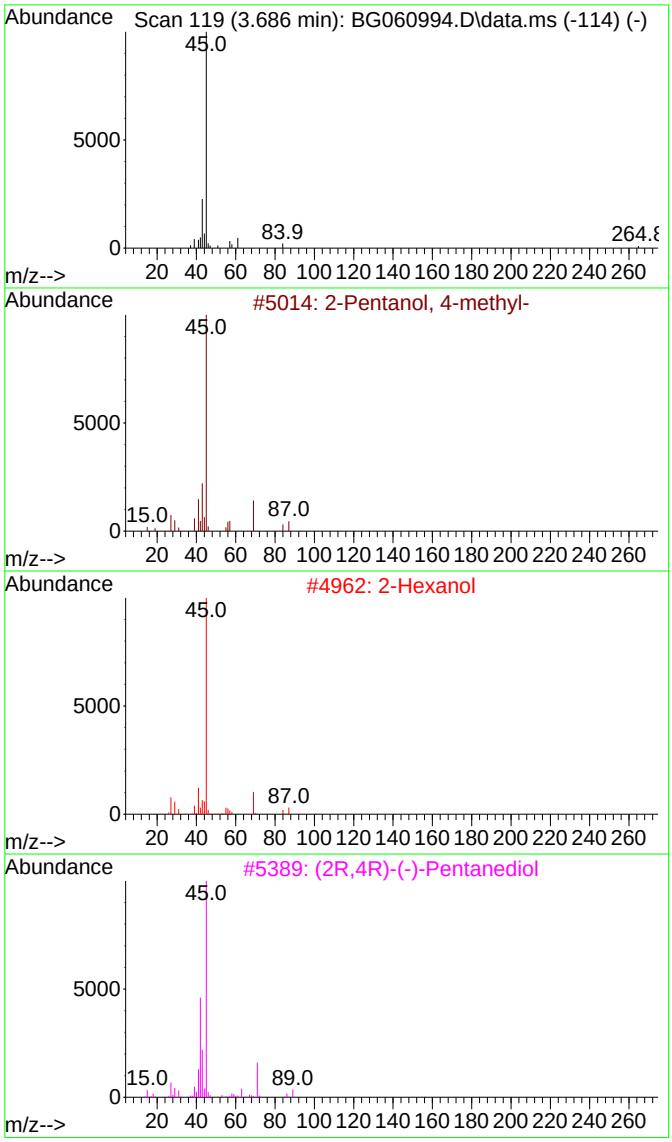
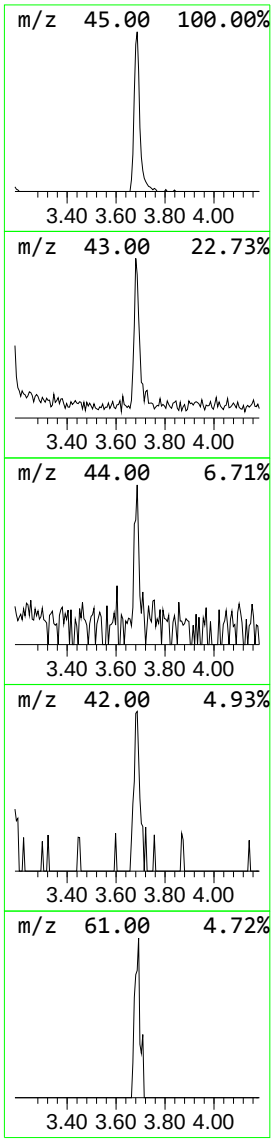
Peak Number 2 2-Pentanol, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.686	4.76 ng	41699	1,4-Dichlorobenzene-d4	7.940

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	56
2	2-Hexanol	102	C6H14O	000626-93-7	40
3	(2R,4R)-(-)-Pentanediol	104	C5H12O2	042075-32-1	40
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
5	Methoxyacetic acid, pentyl ester	160	C8H16O3	168920-35-2	9





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Operator : MA/JU
Sample : P2147-02
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042024.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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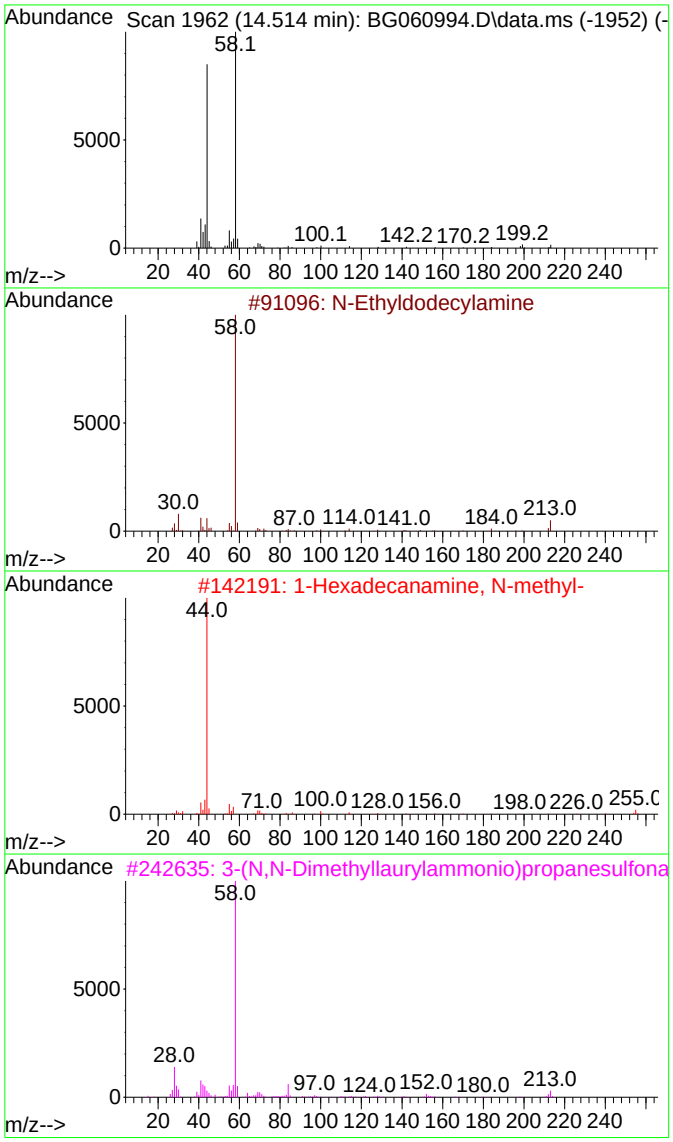
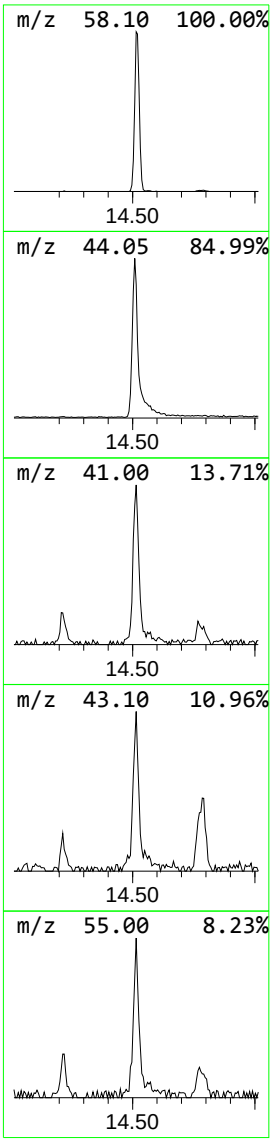
Peak Number 3 unknown14.514 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.514	17.58 ng	305773	Acenaphthene-d10	14.567

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Ethyldodecylamine	213	C14H31N	1000426-51-2	37
2	1-Hexadecanamine, N-methyl-	255	C17H37N	013417-08-8	35
3	3-(N,N-Dimethyllaurylammonio)pro...	335	C17H37NO3S	014933-08-5	32
4	1-Undecanamine, N,N-dimethyl-	199	C13H29N	017373-28-3	32
5	Acetone, 1-[4-(dimethylaminoetho...	221	C13H19NO2	086608-11-9	32





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

TIC Library : C:\Database\NIST20.L
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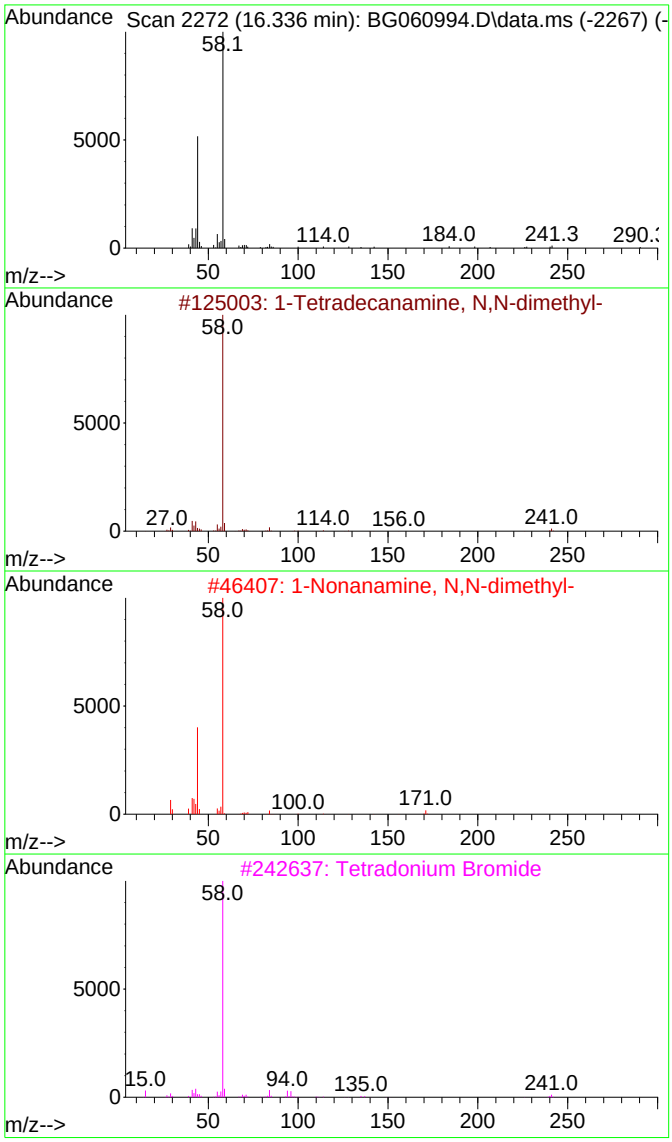
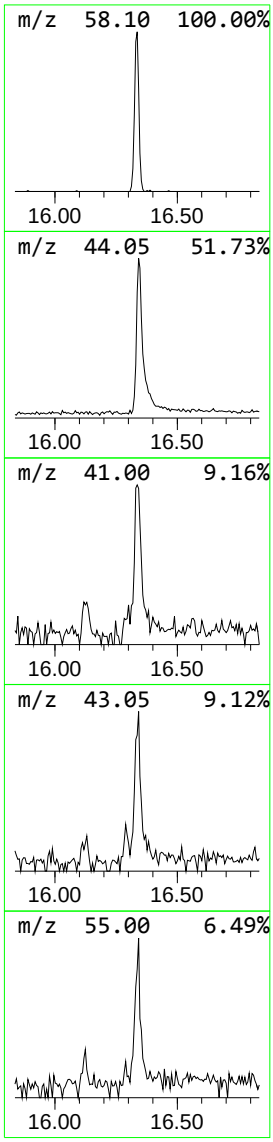
Peak Number 4 1-Tetradecanamine, N,N-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.336	5.07 ng	108776	Phenanthrene-d10	17.317

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	58
2	1-Nonanamine, N,N-dimethyl-	171	C11H25N	017373-27-2	56
3	Tetradonium Bromide	335	C17H38BrN	001119-97-7	50
4	Decane,-1,10-diamino,-N,N,N',N'-...	228	C14H32N2	001938-62-1	50
5	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	50





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Misc :
ALS Vial : 8 Sample Multiplier: 1

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

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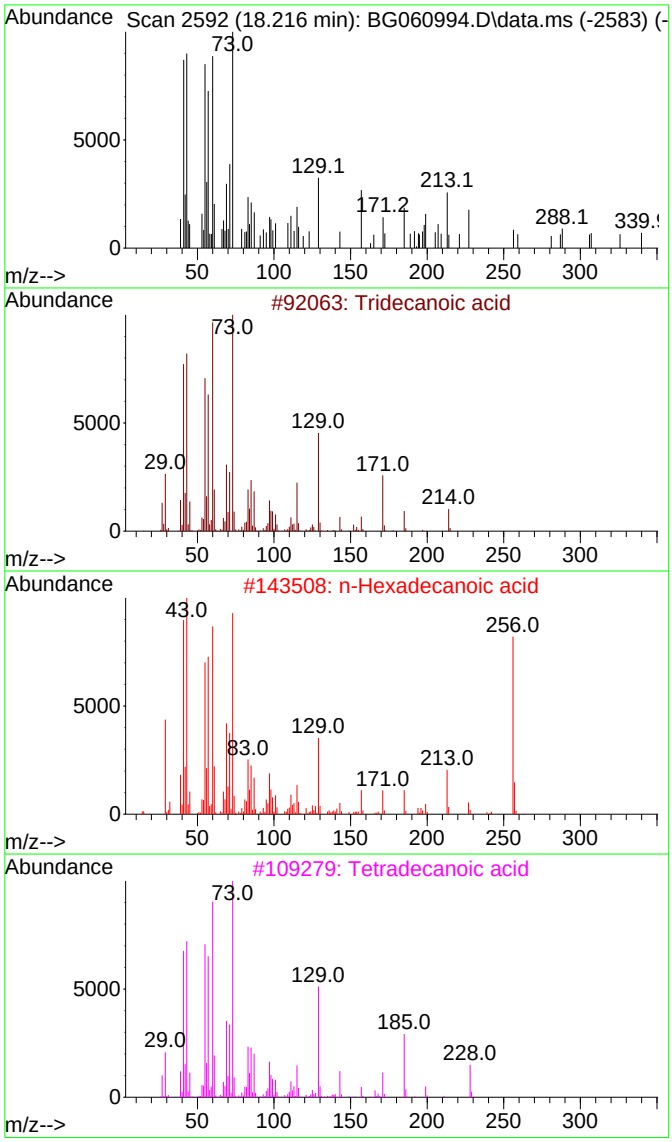
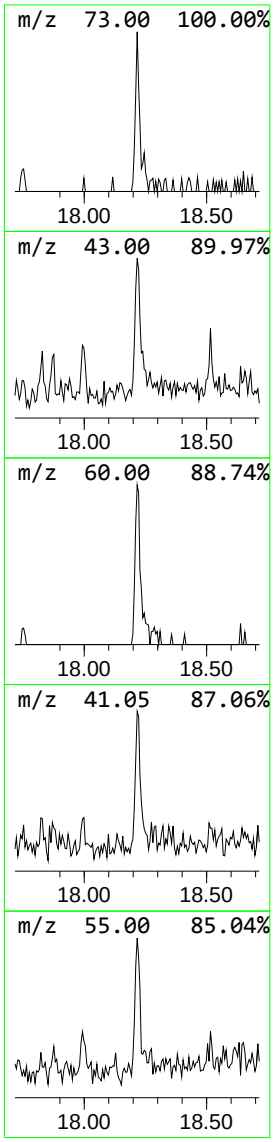
Peak Number 5 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	3.34 ng	71807	Phenanthrene-d10	17.317

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





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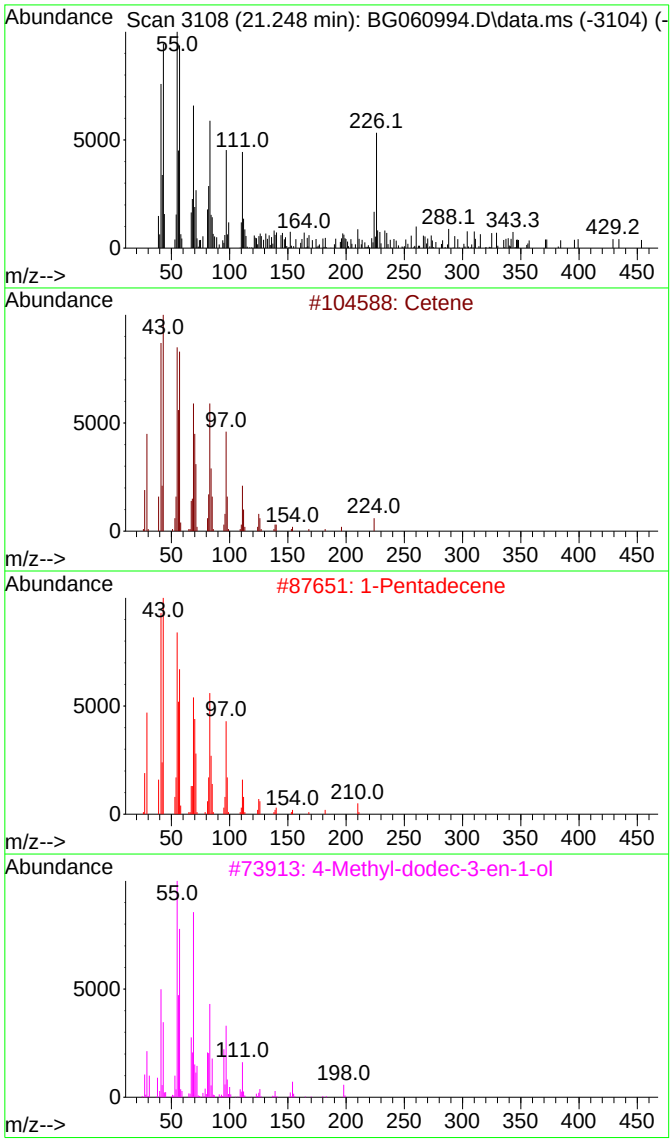
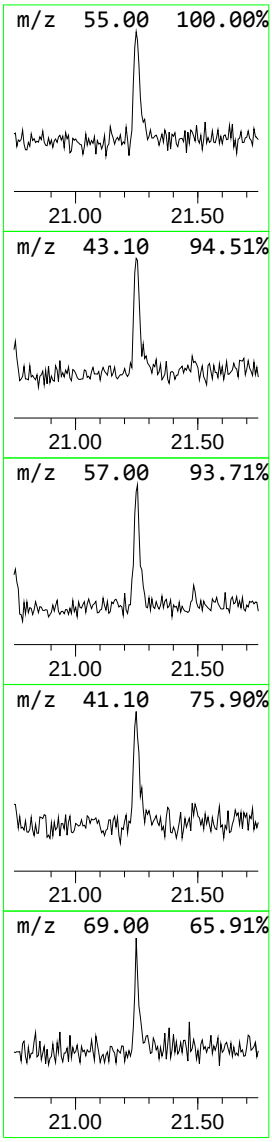
Peak Number 6 Cetene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.248	3.10 ng	83658	Chrysene-d12	21.577

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	78
2	1-Pentadecene	210	C15H30	013360-61-7	49
3	4-Methyl-dodec-3-en-1-ol	198	C13H26O	156992-84-6	46
4	1-Tetradecene	196	C14H28	001120-36-1	46
5	Cyclopentadecane	210	C15H30	000295-48-7	46





Tentatively Identified Compound (LSC) summary

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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...	3.169	5.4	ng	47611	1	7.940	175300	20.0
2-Pentanol, 4-m...	3.686	4.8	ng	41699	1	7.940	175300	20.0
unknown14.514	14.514	17.6	ng	305773	3	14.567	347956	20.0
1-Tetradecanami...	16.336	5.1	ng	108776	4	17.317	429492	20.0
Tridecanoic acid	18.216	3.3	ng	71807	4	17.317	429492	20.0
Cetene	21.248	3.1	ng	83658	5	21.577	540123	20.0