LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110436.D
Acq On : 3 Nov 2018 2:27
Operator : JU/SJ
Sample : J5734-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-21(0-10)

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-BF102318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.293	29	35	47	rVB	347901	456133	23.94%	2.782%
2	5.199	525	529	540	rBV	56700	69954	3.67%	0.427%
3	5.581	590	594	614	rBV	1685168	1737387	91.17%	10.595%
4	6.581	759	764	784	rBV	1654571	1905557	100.00%	11.620%
5	6.728	784	789	792	rBV	2034360	1806778	94.82%	11.018%
6	6.957	824	828	834	rBV	615453	531722	27.90%	3.242%
7	7.110	850	854	858	rBV	1630983	1393363	73.12%	8.497%
8	7.516	919	923	935	rBV	990107	1044754	54.83%	6.371%
9	8.239	1042	1046	1062	rBV	612147	625663	32.83%	3.815%
10	9.310	1224	1228	1237	rBV	2032354	1754357	92.07%	10.698%
11	9.704	1291	1295	1303	rBV	195858	186490	9.79%	1.137%
12	9.998	1341	1345	1358	rVB	616847	589691	30.95%	3.596%
13	10.786	1475	1479	1490	rBV	863115	847555	44.48%	5.168%
14	11.492	1595	1599	1607	rBV	512344	537148	28.19%	3.276%
15	11.992	1681	1684	1688	rBV	23509	21966	1.15%	0.134%
16	12.704	1802	1805	1809	rBV	22808	22618	1.19%	0.138%
17	12.863	1829	1832	1837	rBV	60029	51583	2.71%	0.315%
18	12.939	1837	1845	1849	rVV	25395	33524	1.76%	0.204%
19	13.069	1863	1867	1871	rBV	1629230	1405893	73.78%	8.573%
20	13.539	1941	1947	1952	rBV	159243	165618	8.69%	1.010%
21	13.586	1952	1955	1957	rBV	34387	30459	1.60%	0.186%
22	13.951	2014	2017	2022	rBV	73787	90761	4.76%	0.553%
23	14.133	2044	2048	2055	rBV	430624	460753	24.18%	2.810%
24	14.263	2067	2070	2074	rBV	35636	32437	1.70%	0.198%
25	14.568	2119	2122	2134	rVB	54359	85397	4.48%	0.521%
26	14.886	2173	2176	2181	rVB2	59831	63979	3.36%	0.390%
27	15.239	2232	2236	2240	rVB	71272	87824	4.61%	0.536%
28	15.663	2300	2308	2314	rVB	209401	359312	18.86%	2.191%

Sum of corrected areas: 16398676

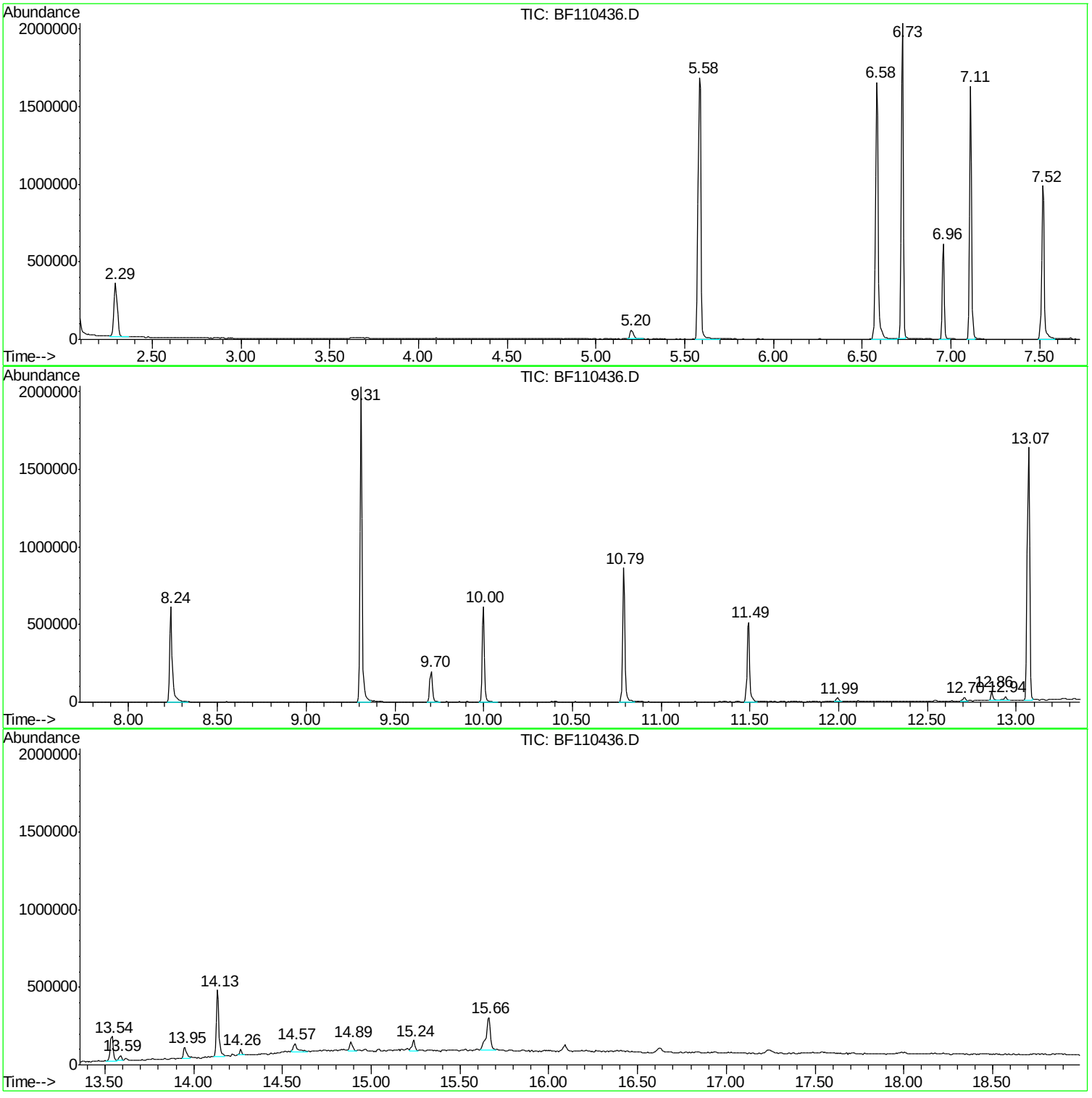
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110436.D
Acq On : 3 Nov 2018 2:27
Operator : JU/SJ
Sample : J5734-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-21(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF110436.D
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Operator : JU/SJ
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Instrument : BNA_F
ClientSampleId : B-21(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

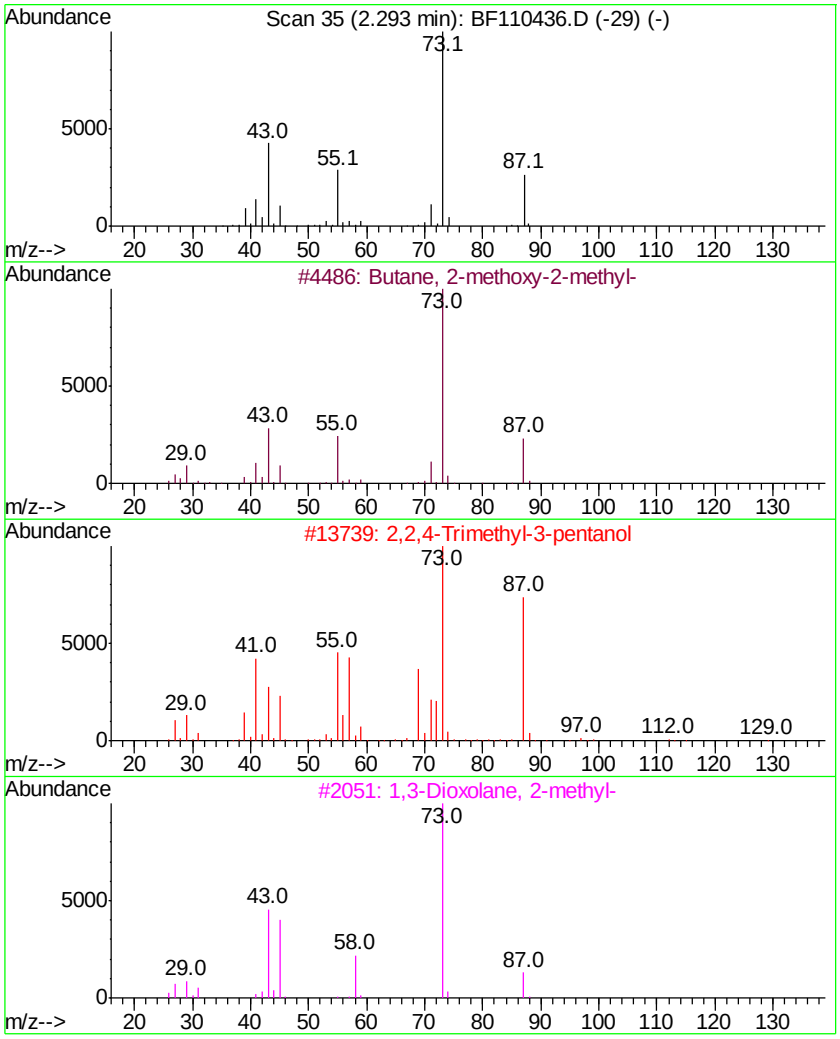
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

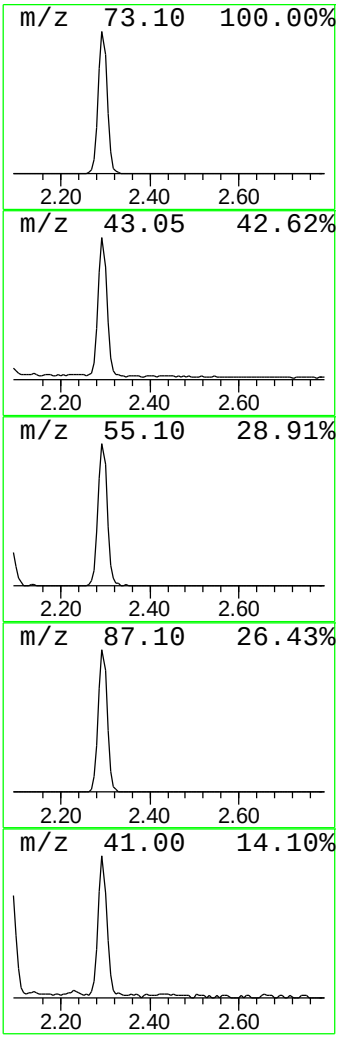
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.29	17.16 ng	456133	1,4-Dichlorobenzene-d4	6.96

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Operator : JU/SJ
Sample : J5734-02
Misc :
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Instrument : BNA_F
ClientSampleId : B-21(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

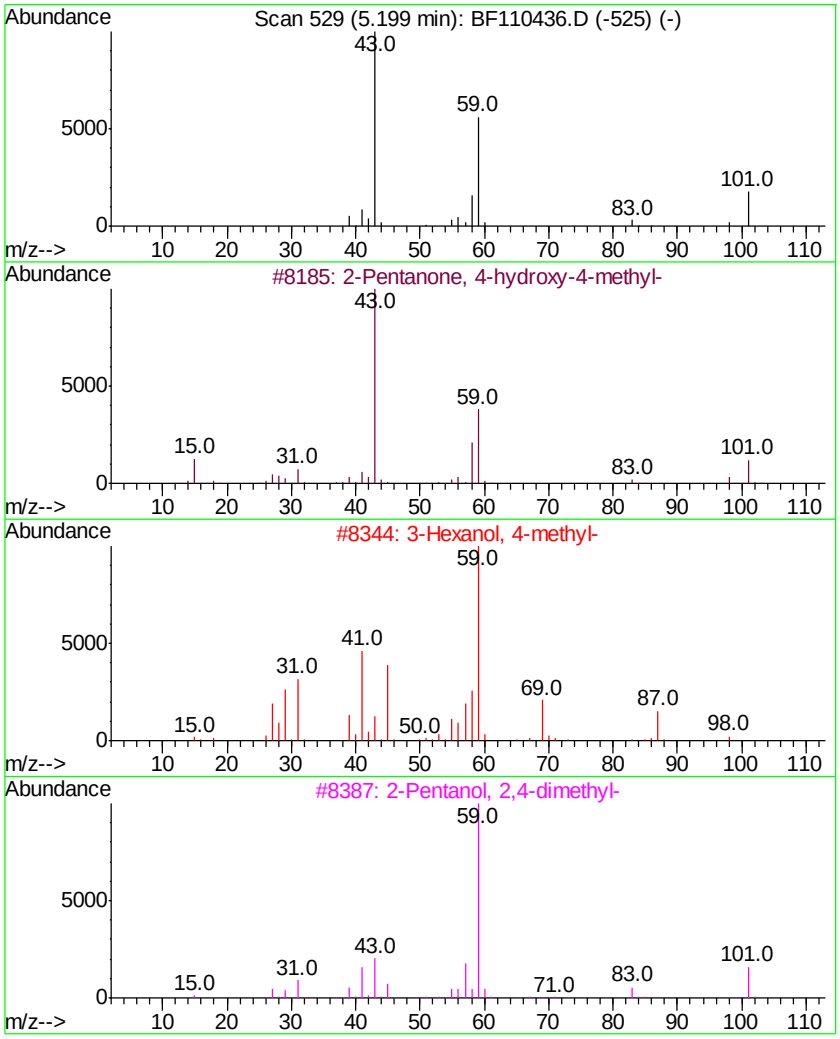
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

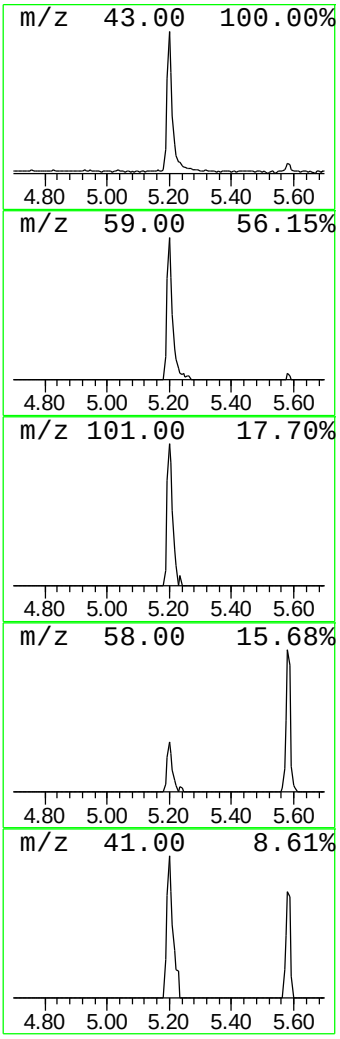
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.63 ng	69954	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	2-Nonanone	142	C9H18O	000821-55-6	9





Library Search Compound Report

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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-21(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

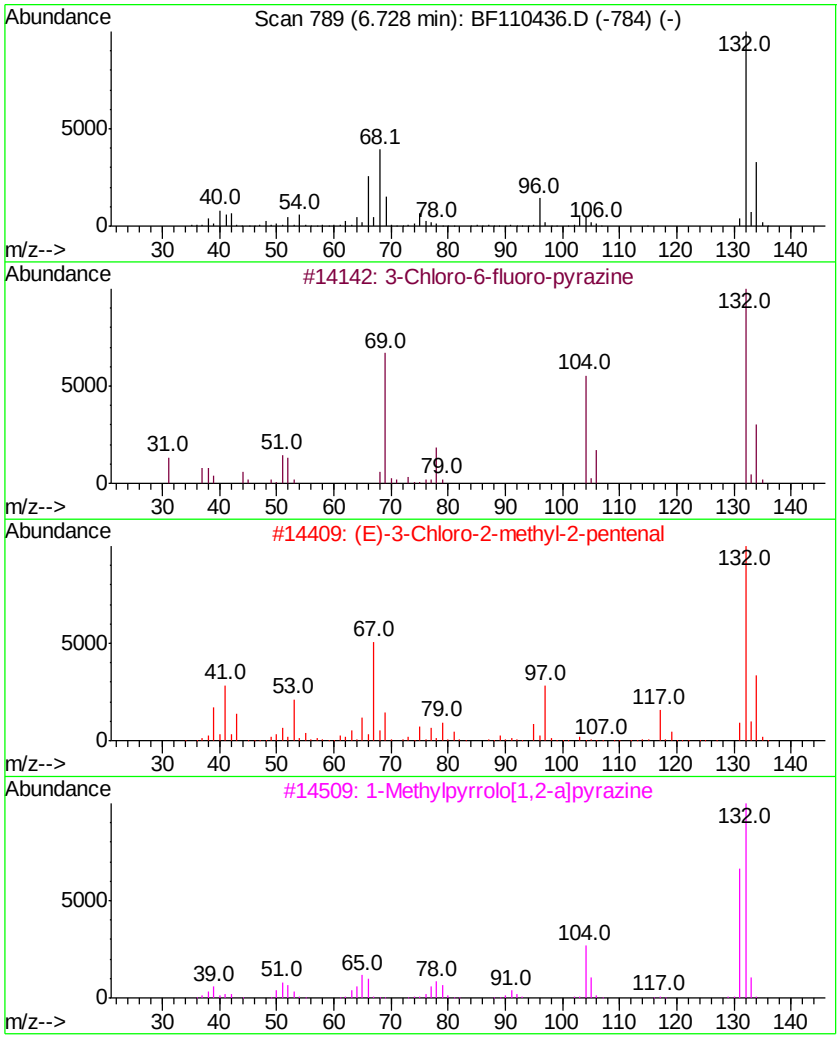
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

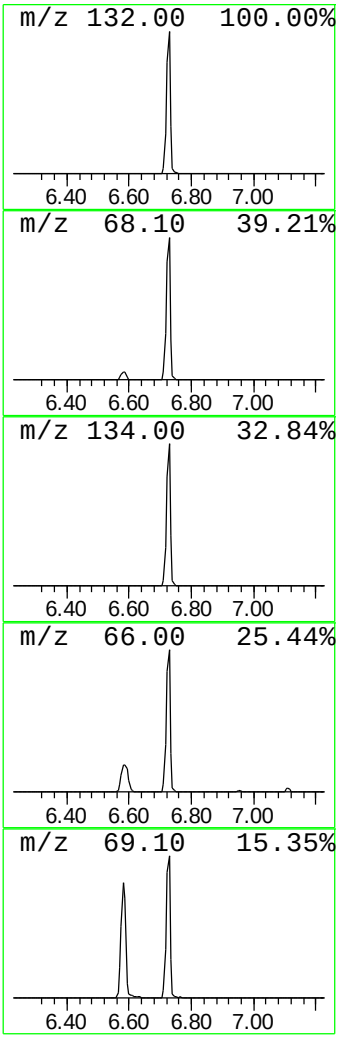
****

Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	67.96 ng	1806780	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-21(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
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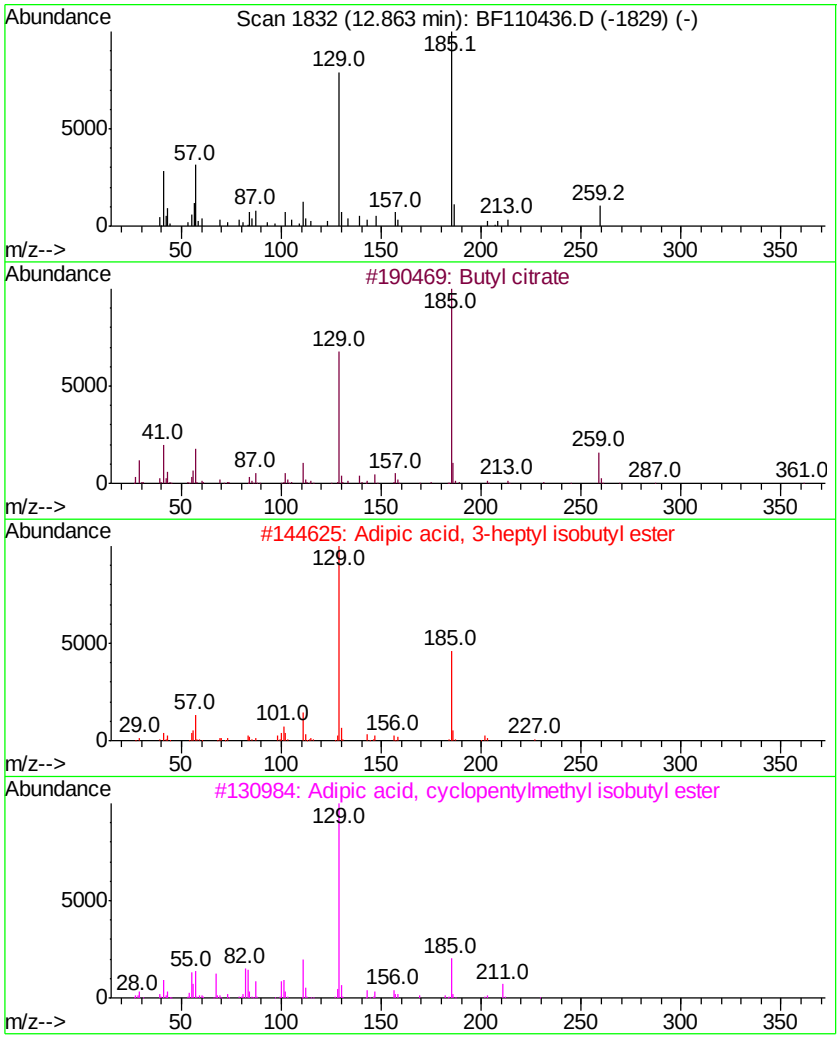
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

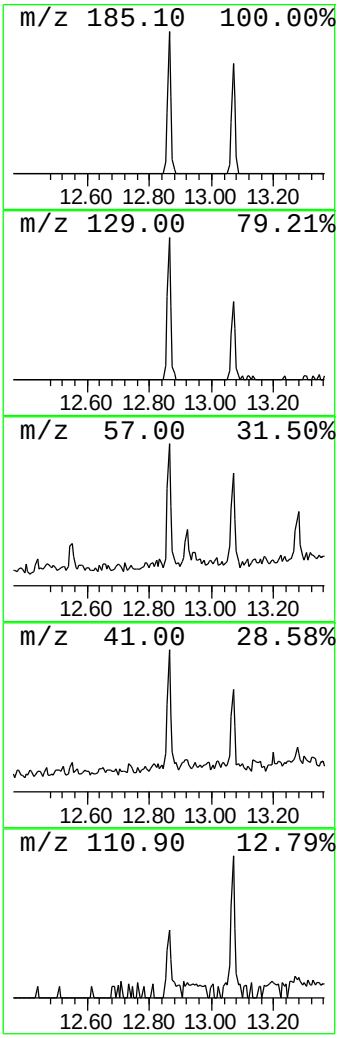
****

Peak Number 5 Butyl citrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.86	2.24 ng	51583	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	90
2	Adipic acid, 3-heptyl isobutyl e...	300	C17H32O4	1000353-64-8	72
3	Adipic acid, cyclopentylmethyl i...	284	C16H28O4	1000324-77-3	72
4	Adipic acid, isobutyl 2-pentyl e...	272	C15H28O4	1000324-15-6	72
5	Adipic acid, butyl 2-methylpent-...	286	C16H30O4	1000353-55-8	72





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Operator : JU/SJ
Sample : J5734-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-21(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
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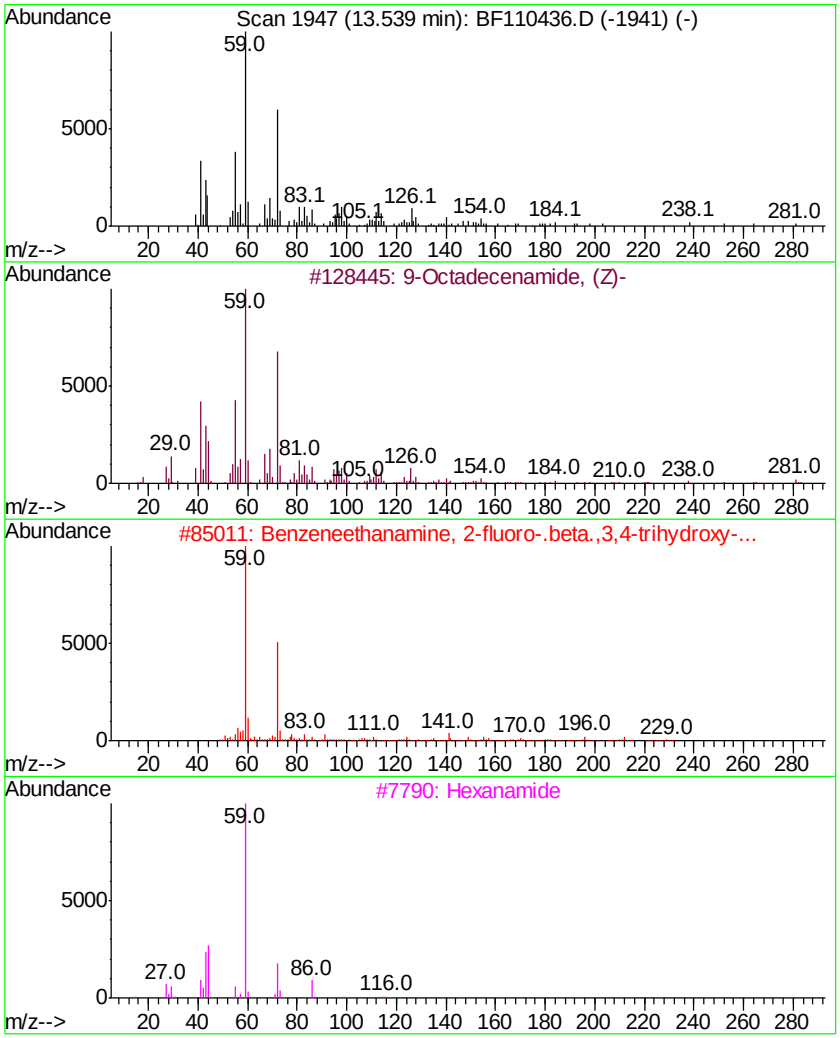
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

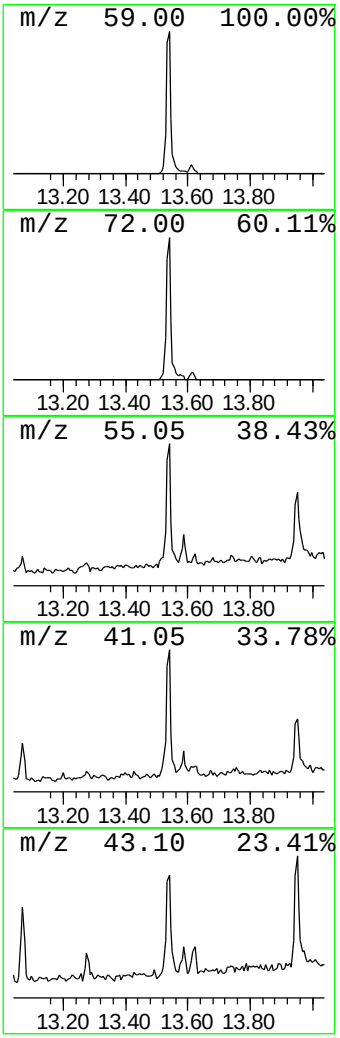
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	7.19 ng	165618	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59
3	Hexanamide	115	C6H13NO	000628-02-4	47
4	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	43
5	1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	43





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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-21(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

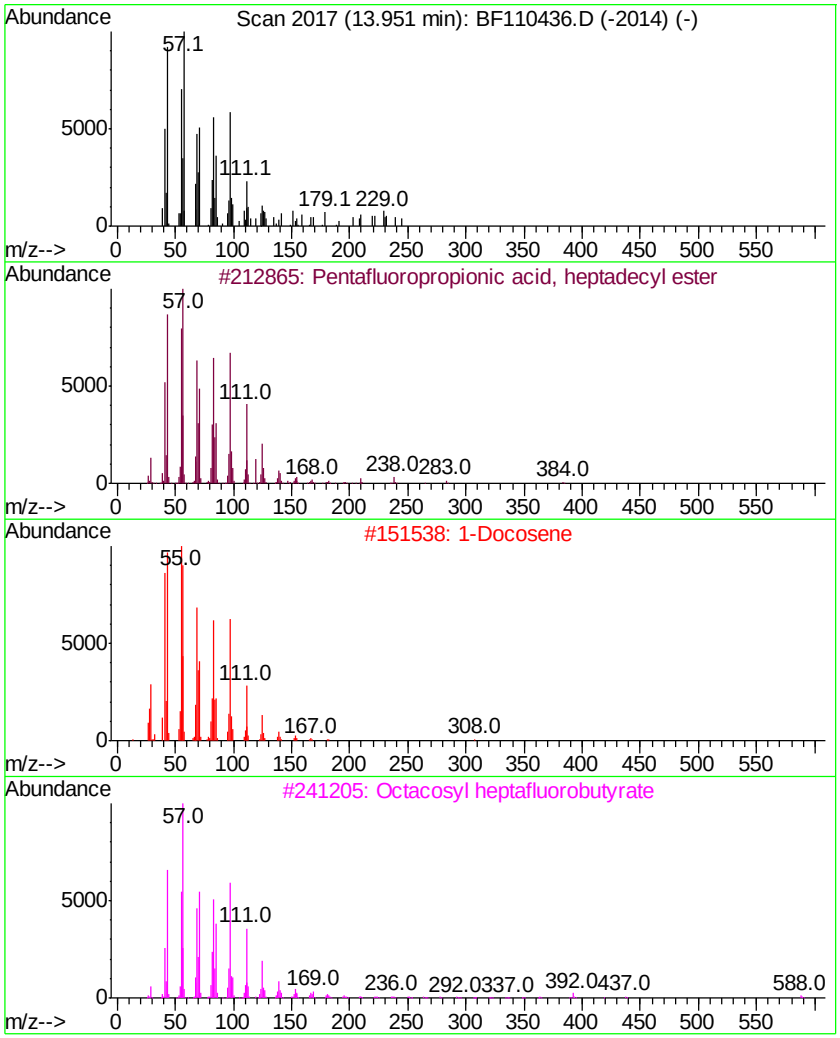
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

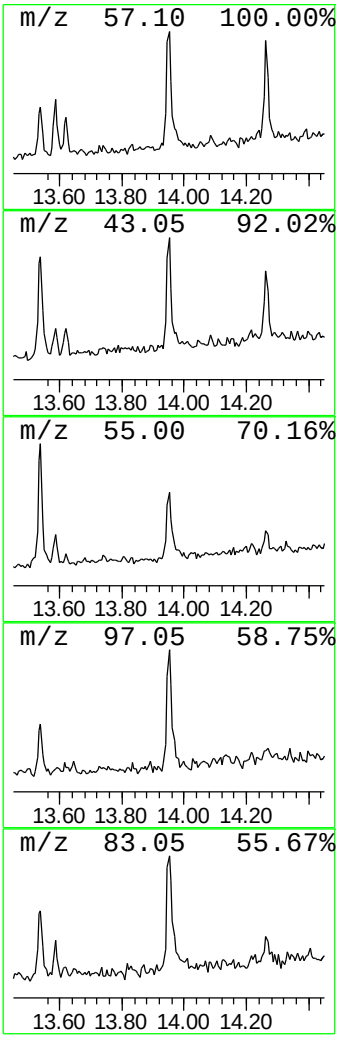
****

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.94 ng	90761	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	83
2	1-Docosene	308	C22H44	001599-67-3	70
3	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	68
4	Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	64
5	1-Heptacosanol	396	C27H56O	002004-39-9	62





Library Search Compound Report

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ClientSampleId : B-21(0-10)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

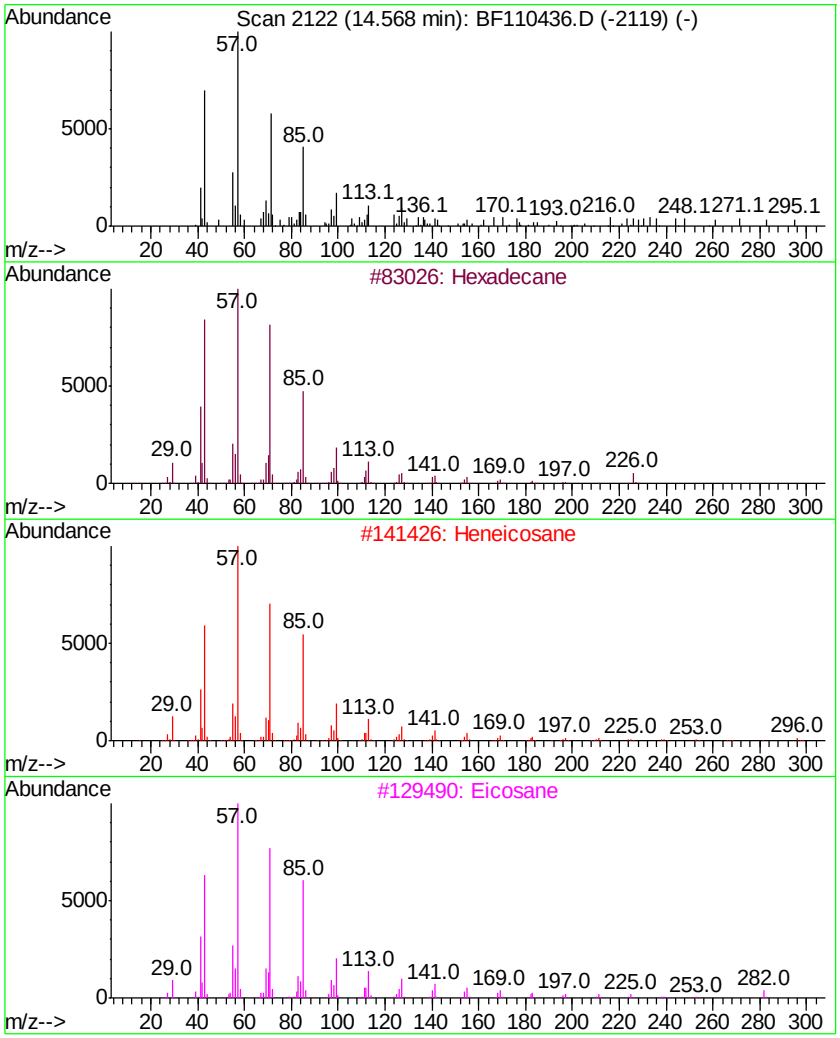
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

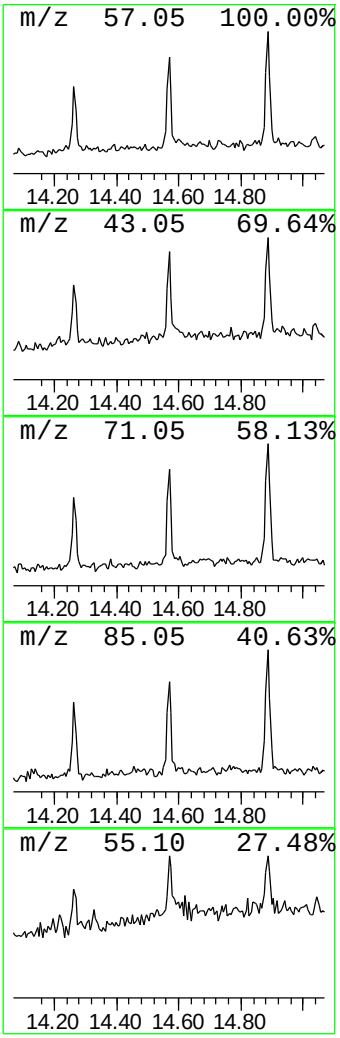
****

Peak Number 8 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	3.71 ng	85397	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Heneicosane	296	C21H44	000629-94-7	58
3	Eicosane	282	C20H42	000112-95-8	52
4	Octacosane	394	C28H58	000630-02-4	52
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	52





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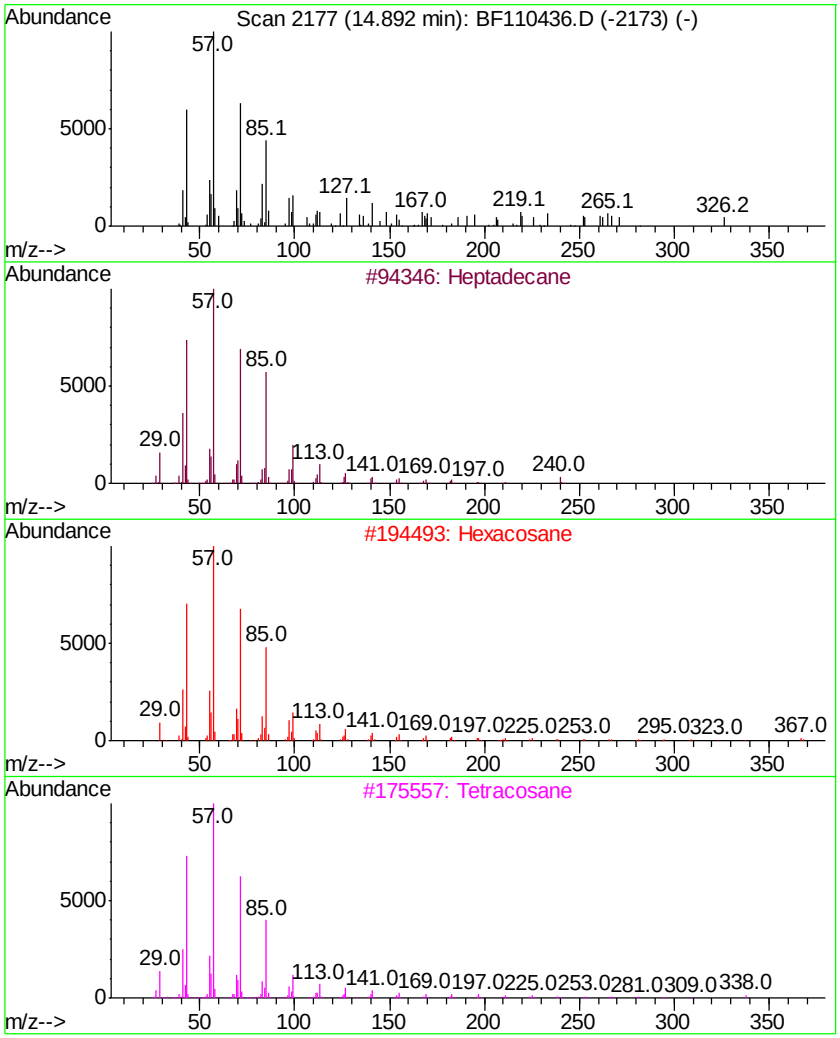
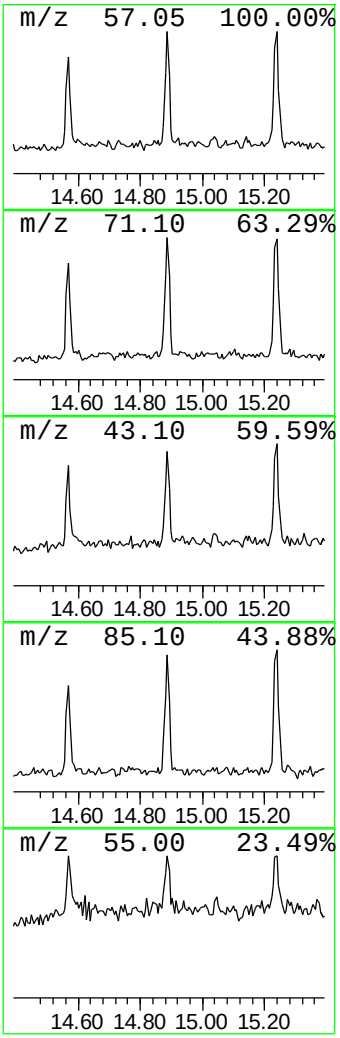
****

Peak Number 9 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.78 ng	63979	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	83
2	Hexacosane	366	C26H54	000630-01-3	83
3	Tetracosane	338	C24H50	000646-31-1	80
4	Eicosane	282	C20H42	000112-95-8	80
5	Heneicosane	296	C21H44	000629-94-7	80





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ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-21(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

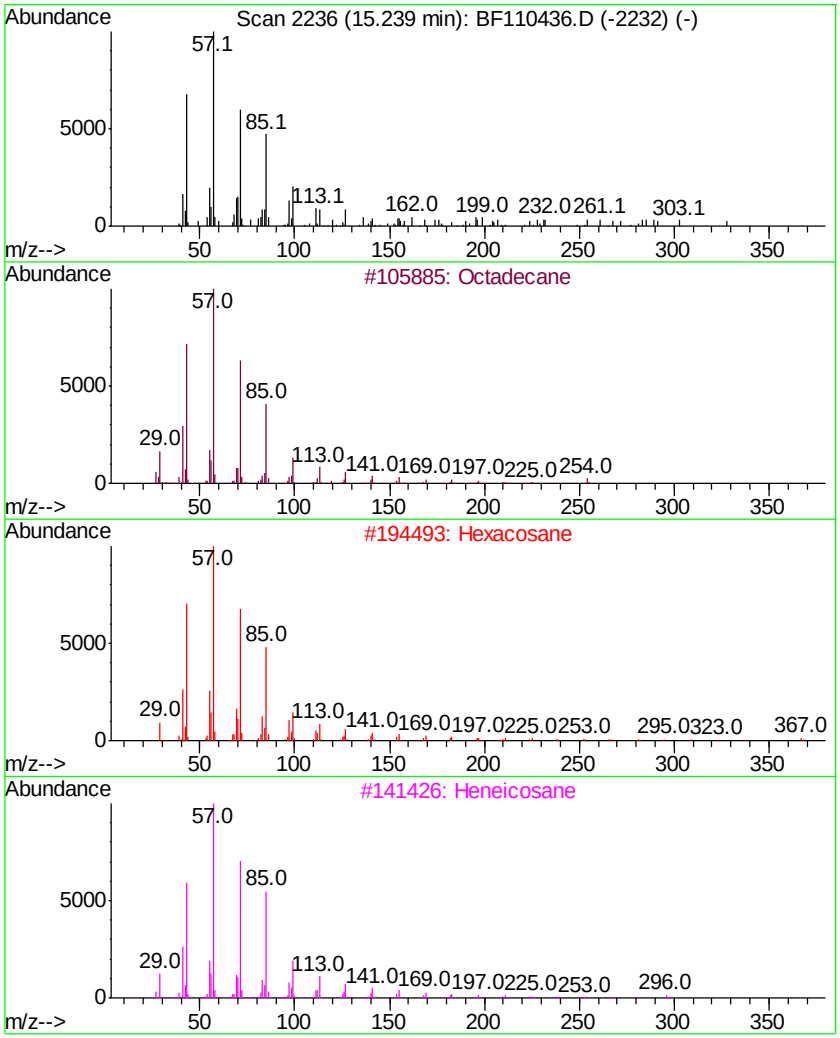
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

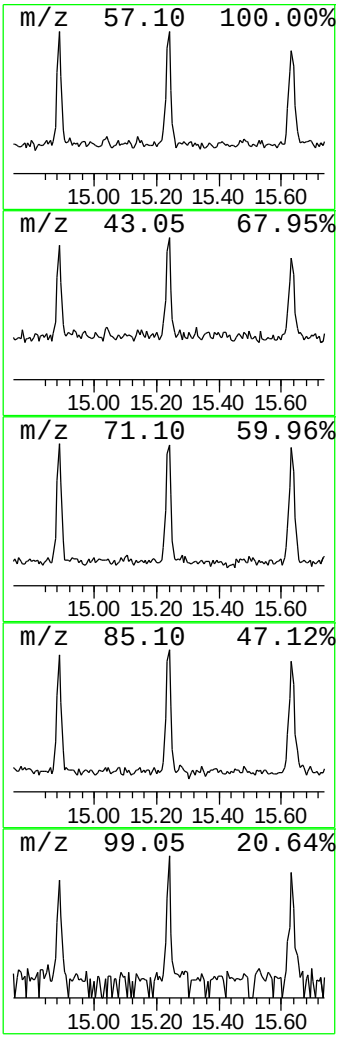
****

Peak Number 10 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	4.89 ng	87824	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	92
2	Hexacosane	366	C26H54	000630-01-3	74
3	Heneicosane	296	C21H44	000629-94-7	74
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	72
5	Tetratetracontane	619	C44H90	007098-22-8	72





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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
Butane, 2-methoxy...	2.29	17.2	ng	456133	1	6.96	531722	20.0
2-Pentanone, 4-hy...	5.20	2.6	ng	69954	1	6.96	531722	20.0
unknown6.73	6.73	68.0	ng	1806780	1	6.96	531722	20.0
Butyl citrate	12.86	2.2	ng	51583	5	14.13	460753	20.0
9-Octadecenamide,...	13.54	7.2	ng	165618	5	14.13	460753	20.0
Pentafluoropropio...	13.95	3.9	ng	90761	5	14.13	460753	20.0
Hexadecane	14.57	3.7	ng	85397	5	14.13	460753	20.0
Heptadecane	14.89	2.8	ng	63979	5	14.13	460753	20.0
Octadecane	15.24	4.9	ng	87824	6	15.66	359312	20.0