LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112454.D
Acq On : 7 Feb 2019 22:32
Operator : JU/SJ
Sample : K1396-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 23935

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-BF012519.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	2.116	3	5	10	rVB	101834	113225	4.32%	0.429%
2	3.904	304	309	320	rBV	149233	212949	8.12%	0.806%
3	5.057	501	505	511	rBV	80536	110150	4.20%	0.417%
4	5.475	572	576	596	rBV	2240734	2345915	89.47%	8.880%
5	6.487	744	748	765	rBV	2313921	2519547	96.10%	9.537%
6	6.610	765	769	777	rVV	3035343	2621915	100.00%	9.924%
7	6.834	803	807	814	rBV	853065	755201	28.80%	2.859%
8	6.898	815	818	825	rVV	90088	140976	5.38%	0.534%
9	6.987	829	833	848	rVB	2121962	1975904	75.36%	7.479%
10	7.222	870	873	878	rBV2	16432	29823	1.14%	0.113%
11	7.398	898	903	914	rBV	1483219	1547474	59.02%	5.857%
12	8.116	1021	1025	1033	rBV	947287	911854	34.78%	3.452%
13	8.545	1092	1098	1106	rBV2	54600	85088	3.25%	0.322%
14	9.186	1203	1207	1217	rBV	2809403	2381102	90.82%	9.013%
15	9.581	1270	1274	1280	rBV	207418	201705	7.69%	0.763%
16	9.792	1307	1310	1314	rVB	33171	29947	1.14%	0.113%
17	9.869	1319	1323	1330	rVB	1112227	997574	38.05%	3.776%
18	10.122	1361	1366	1369	rBV5	22056	35318	1.35%	0.134%
19	10.292	1393	1395	1398	rVB	72923	55188	2.10%	0.209%
20	10.504	1428	1431	1435	rBV4	31959	42981	1.64%	0.163%
21	10.663	1454	1458	1467	rBV	1443554	1395171	53.21%	5.281%
22	10.763	1473	1475	1483	rBV	93902	115200	4.39%	0.436%
23	10.910	1497	1500	1505	rVB6	24394	29378	1.12%	0.111%
24	10.957	1505	1508	1512	rBV	31842	42995	1.64%	0.163%
25	11.086	1527	1530	1532	rBV	71196	64286	2.45%	0.243%
26	11.216	1549	1552	1554	rBV	85774	78184	2.98%	0.296%
27	11.245	1554	1557	1563	rVB2	103231	125068	4.77%	0.473%
28	11.357	1572	1576	1579	rBV	995281	889621	33.93%	3.367%
29	11.380	1579	1580	1587	rVB	164722	157007	5.99%	0.594%
30	11.522	1602	1604	1608	rBV4	62109	64028	2.44%	0.242%
31	11.592	1614	1616	1619	rVB3	47867	43640	1.66%	0.165%
32	11.639	1621	1624	1627	rBV2	81549	85341	3.25%	0.323%
33	11.686	1630	1632	1637	rVB5	44299	55174	2.10%	0.209%
34	11.804	1650	1652	1654	rBV2	61364	58328	2.22%	0.221%

LSC Area Percent Report

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Integrator: RTE
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.880	1662	1665	1667	rBV	240177	222425	8.48%	0.842%
36	11.939	1672	1675	1677	rBV	102956	101688	3.88%	0.385%
37	12.022	1686	1689	1691	rBV2	53933	54306	2.07%	0.206%
38	12.051	1691	1694	1696	rBV	111376	129811	4.95%	0.491%
39	12.333	1739	1742	1744	rBV	192049	206793	7.89%	0.783%
40	12.439	1757	1760	1763	rBV	179143	226576	8.64%	0.858%
41	12.575	1780	1783	1790	rBV2	519152	614461	23.44%	2.326%
42	12.780	1816	1818	1820	rBV3	169486	174633	6.66%	0.661%
43	12.804	1820	1822	1825	rVV2	375348	377051	14.38%	1.427%
44	12.839	1826	1828	1831	rVV	176381	194090	7.40%	0.735%
45	12.939	1840	1845	1849	rBV	1945468	2111847	80.55%	7.994%
46	13.163	1881	1883	1886	rBV	249568	252872	9.64%	0.957%
47	13.416	1924	1926	1929	rVB	332481	274817	10.48%	1.040%
48	14.004	2024	2026	2029	rBV	582946	497145	18.96%	1.882%
49	15.480	2275	2277	2282	rVB	548592	663274	25.30%	2.511%

Sum of corrected areas: 26419046

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BNA_F
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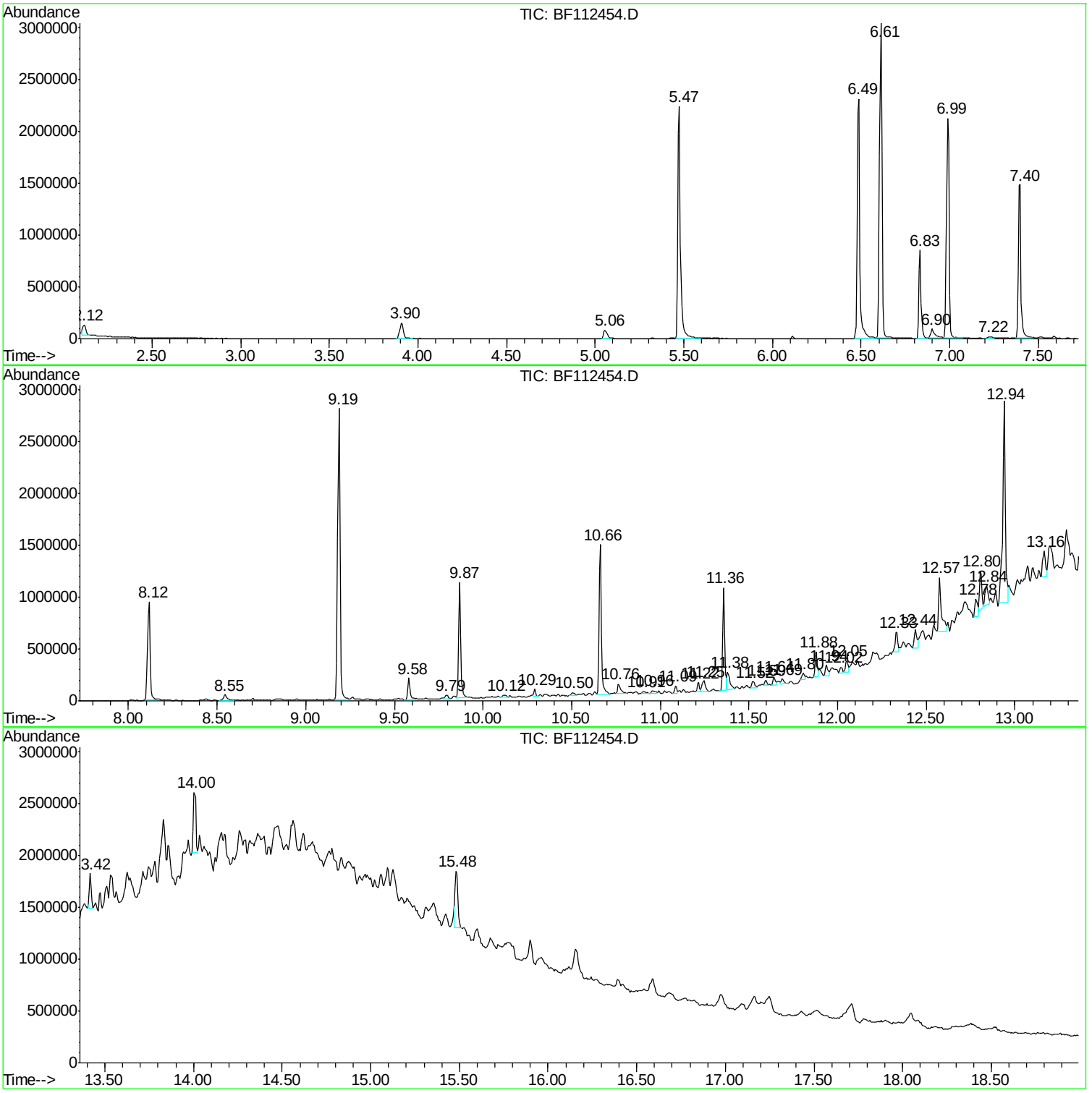
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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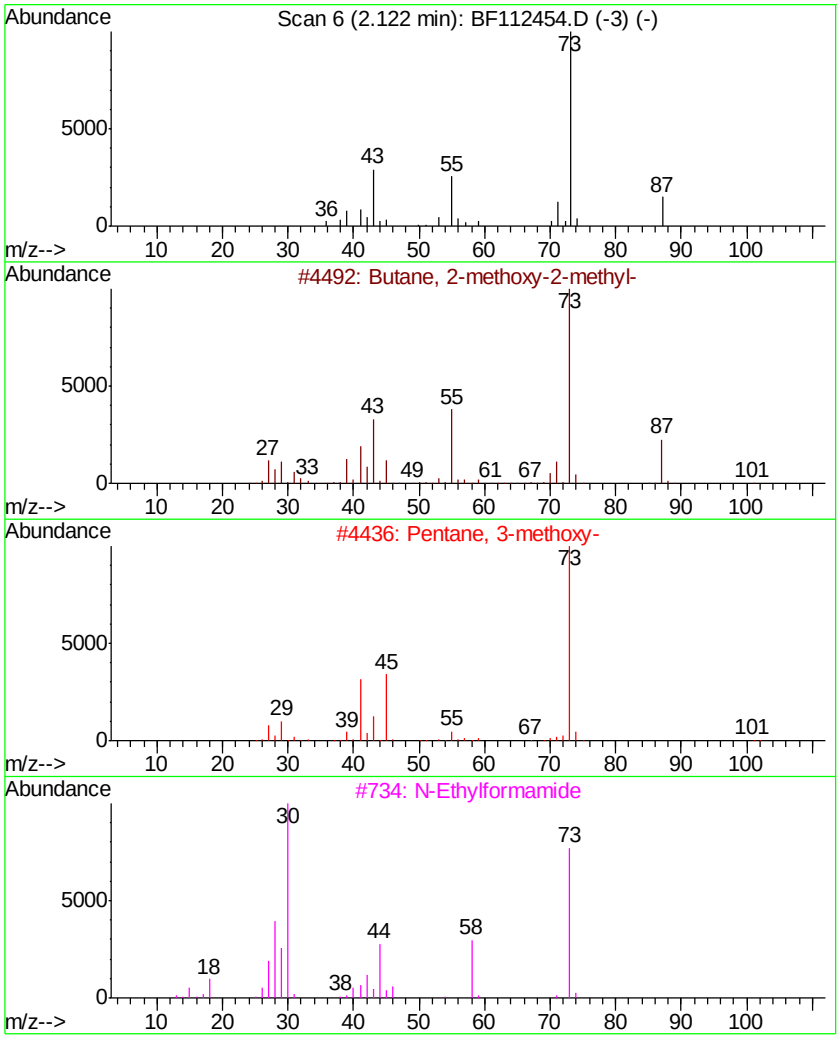
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

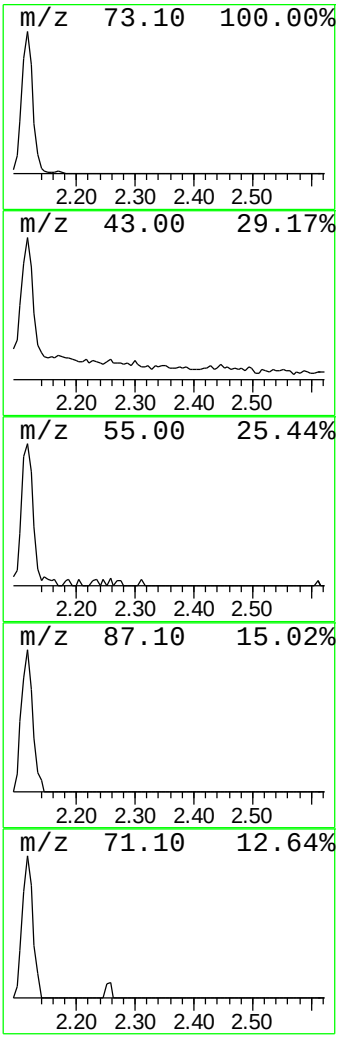
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	3.00 ng	113225	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	1000186-02-3	9





Library Search Compound Report

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Instrument : BNA_F
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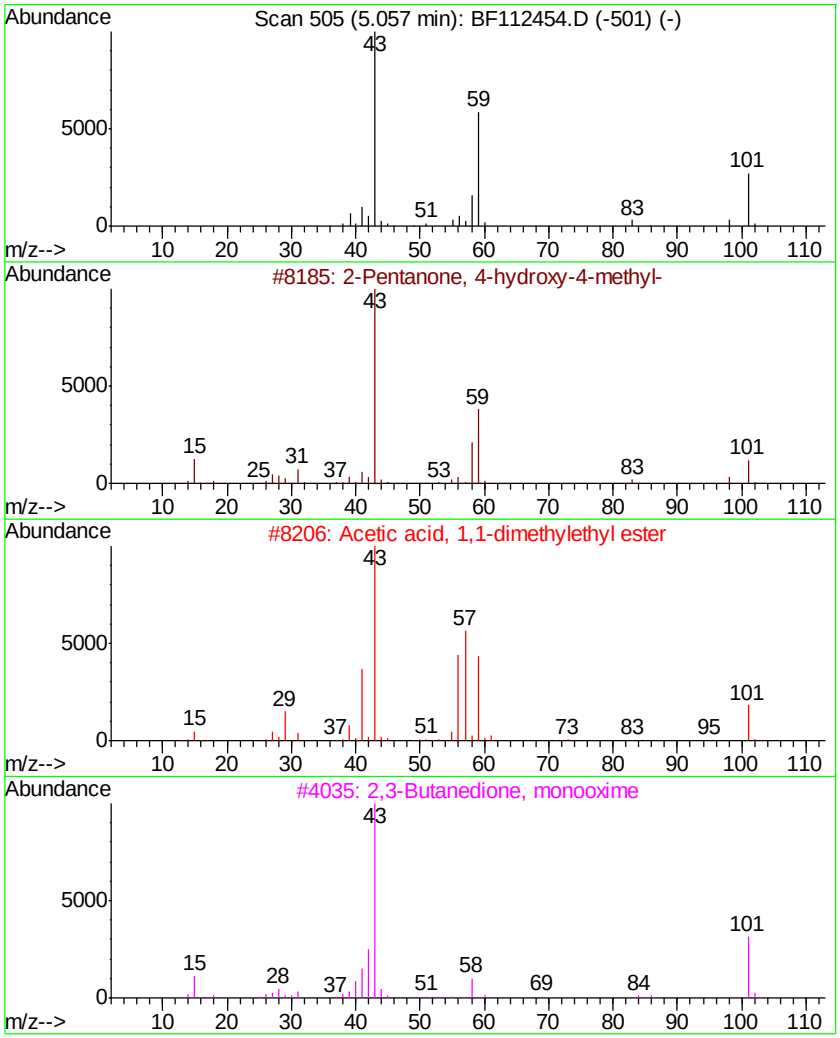
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

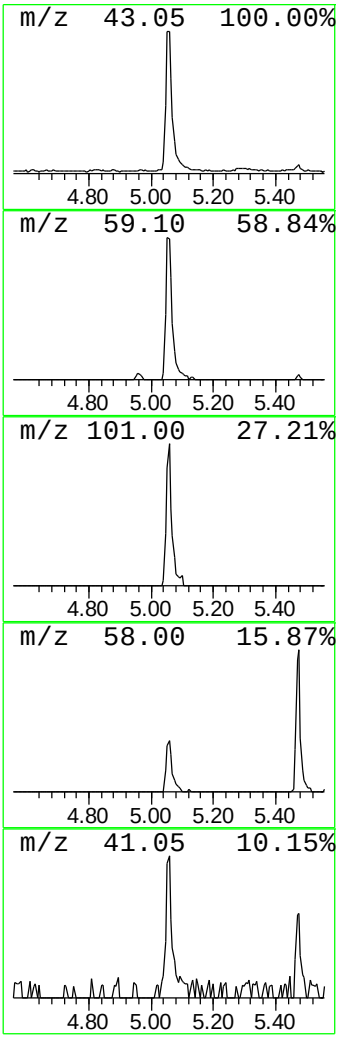
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	2.92 ng	110150	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Data File : BF112454.D
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Operator : JU/SJ
Sample : K1396-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 23935

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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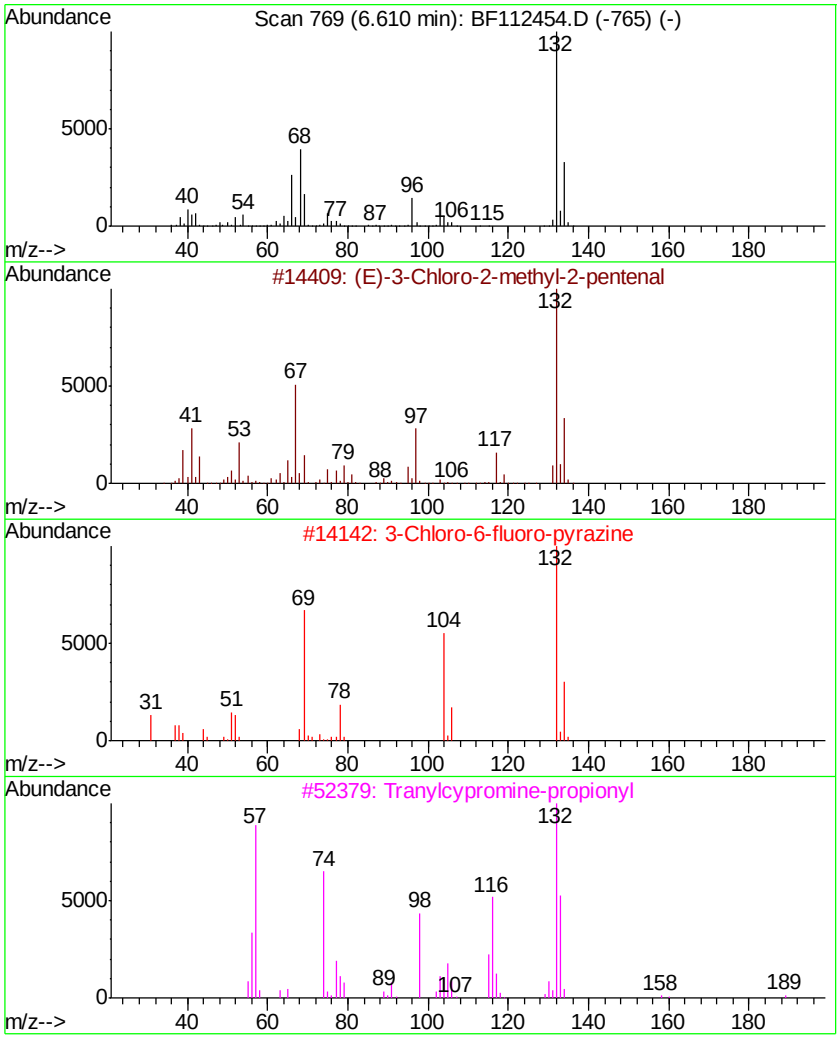
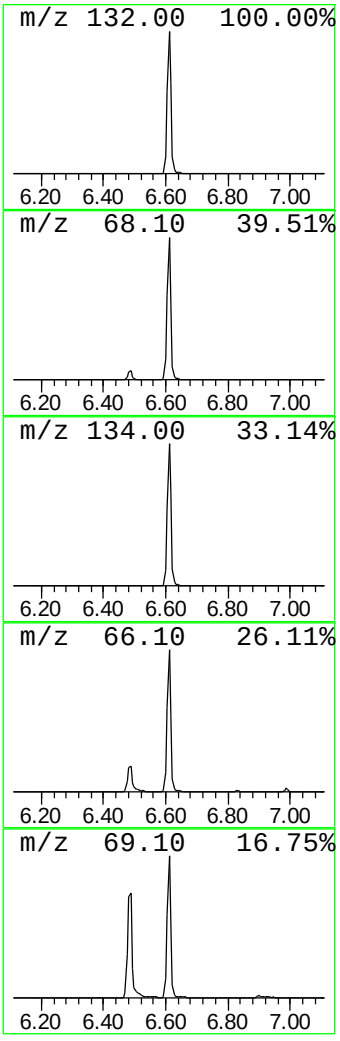
****

Peak Number 4 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	69.44 ng	2621920	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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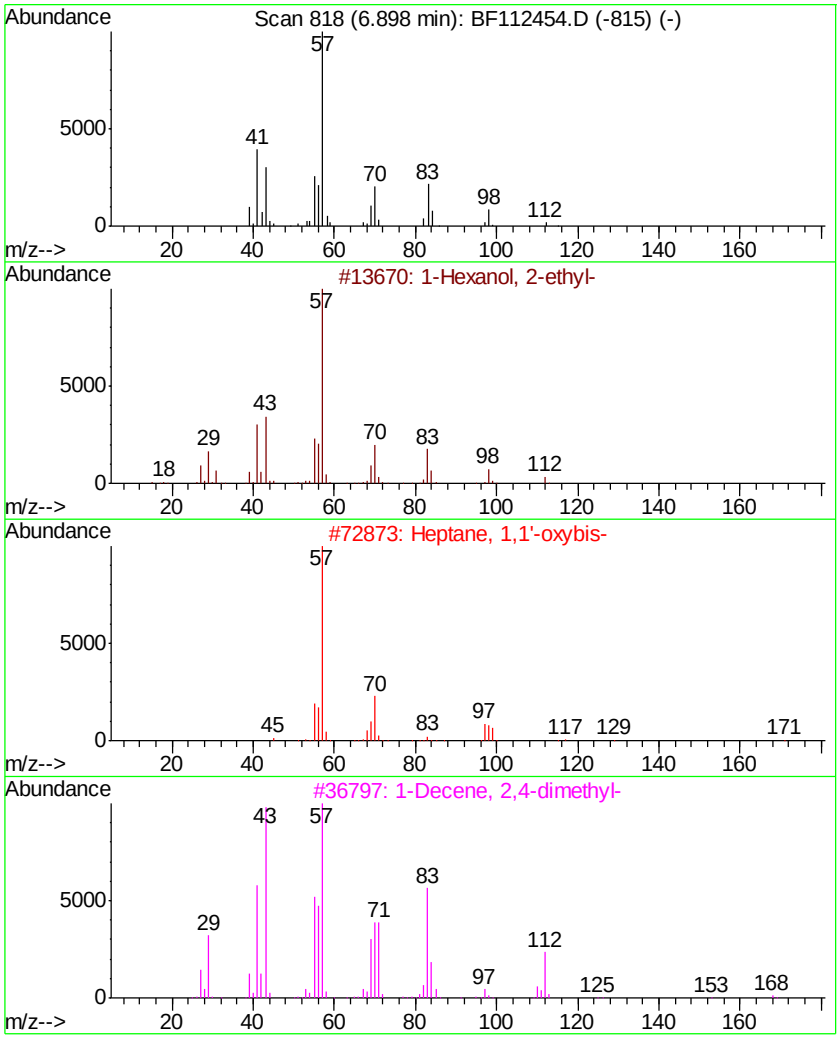
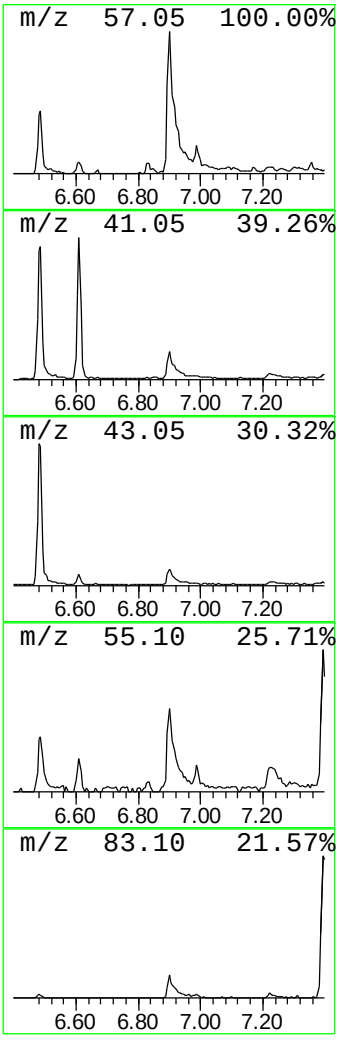
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.90	3.73 ng	140976	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50
4	2-Decene, 5-methyl-, (Z)-	154	C11H22	074645-86-6	47
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47





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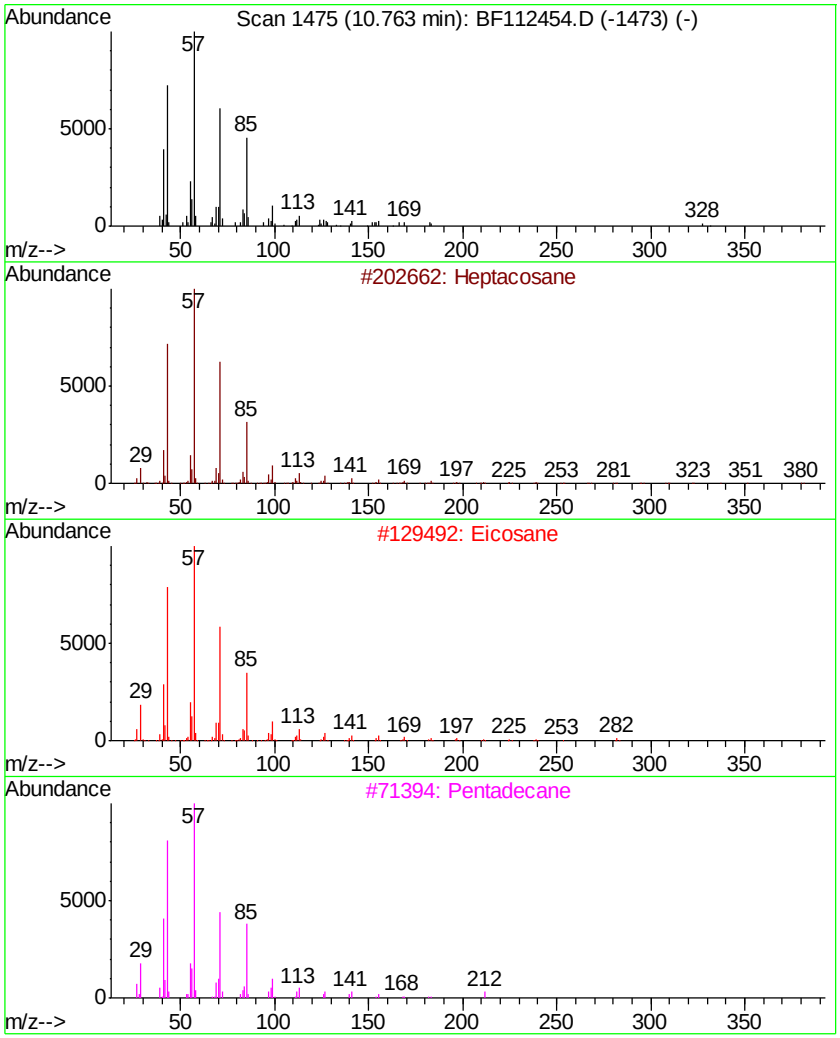
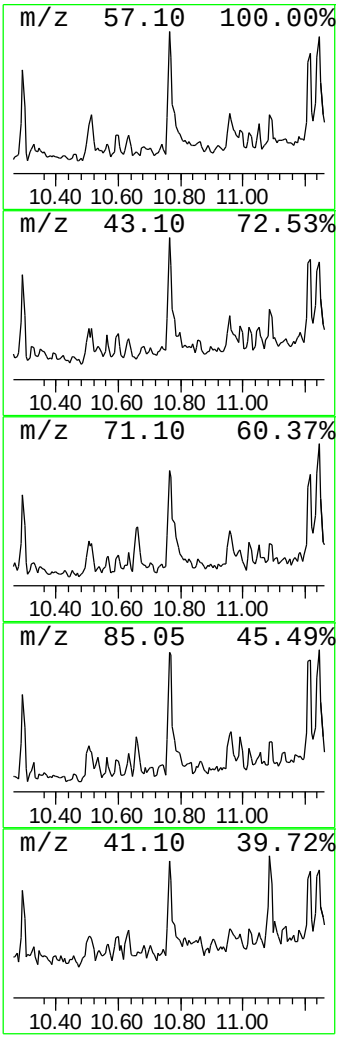
****

Peak Number 7 Heptacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	2.59 ng	115200	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Eicosane	282	C20H42	000112-95-8	87
3	Pentadecane	212	C15H32	000629-62-9	86
4	Tridecane, 7-propyl-	226	C16H34	055045-09-5	86
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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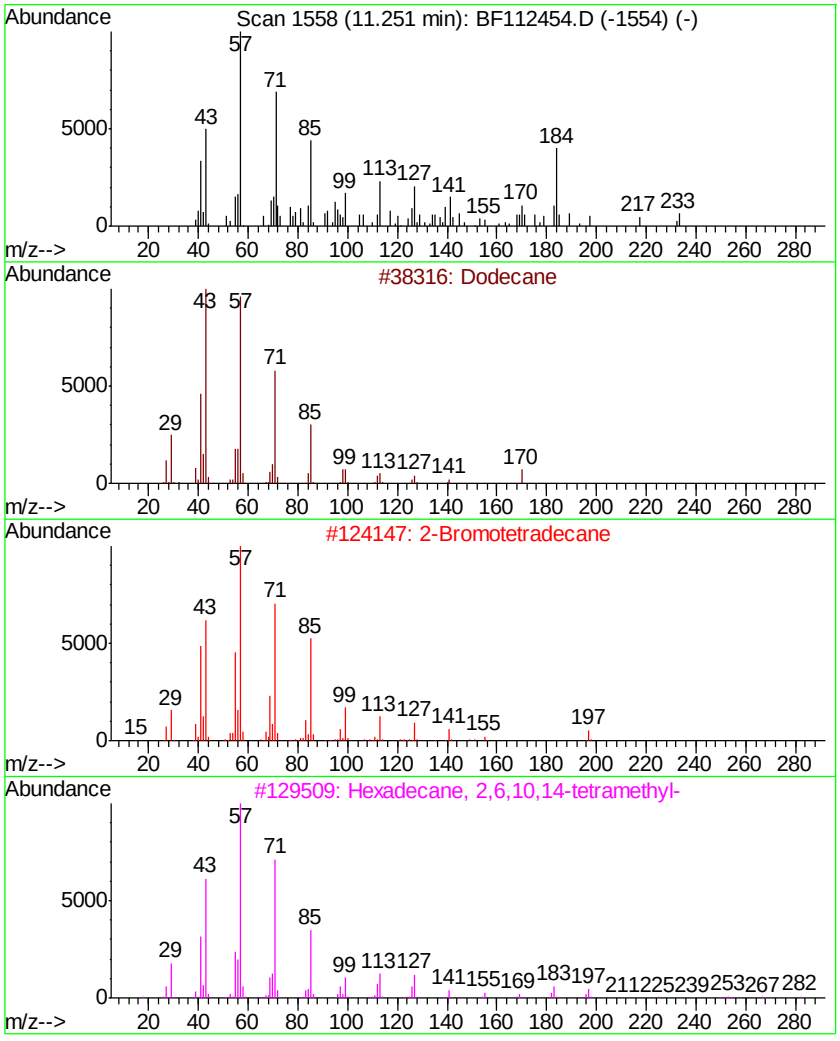
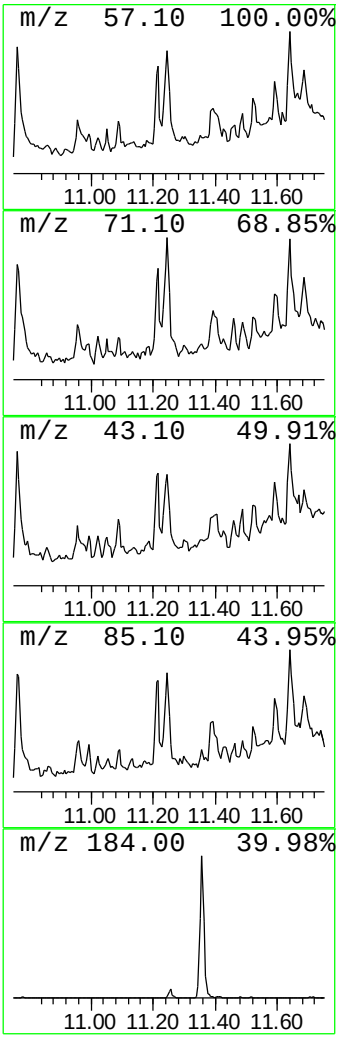
Peak Number 8 Dodecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.25	2.81 ng	125068	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	87
2	2-Bromotetradecane	276	C14H29Br	074036-95-6	87
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	87
4	Hentriacontane	437	C31H64	000630-04-6	86
5	Triacontane	422	C30H62	000638-68-6	86





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

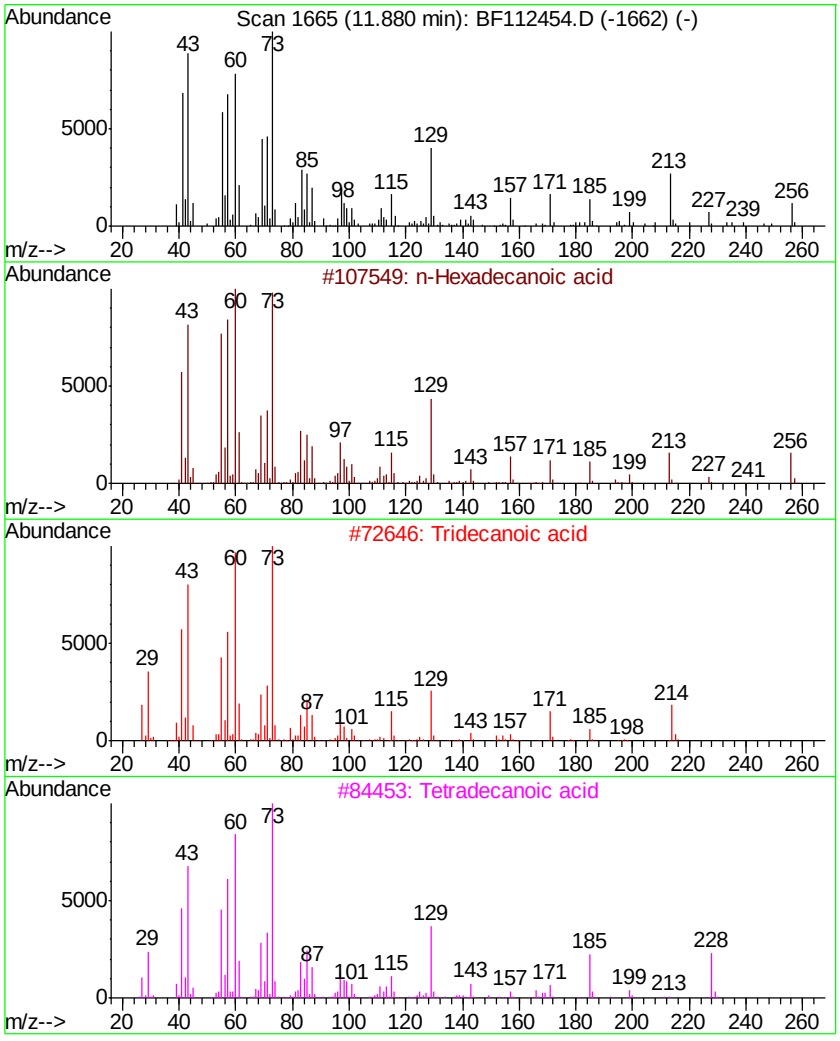
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

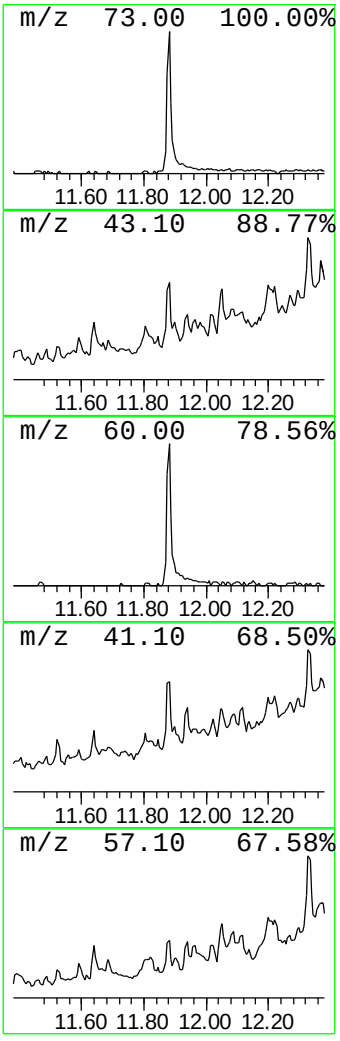
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	5.00 ng	222425	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Sample : K1396-01
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Instrument : BNA_F
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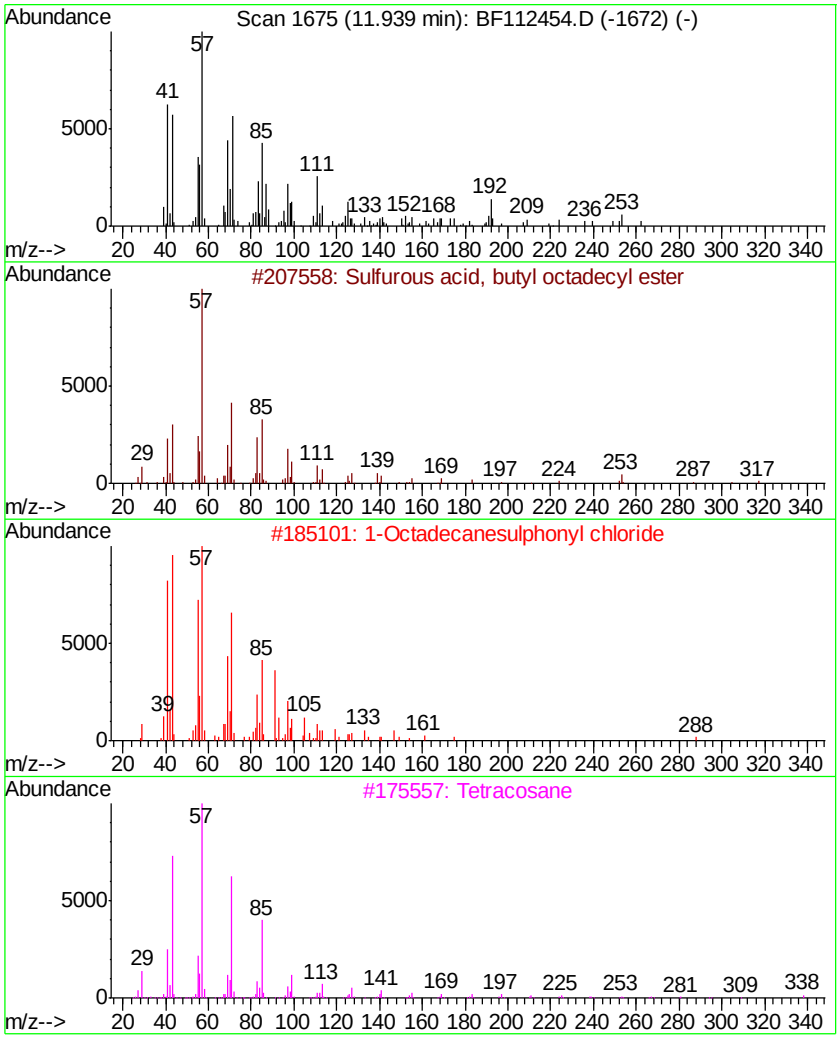
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

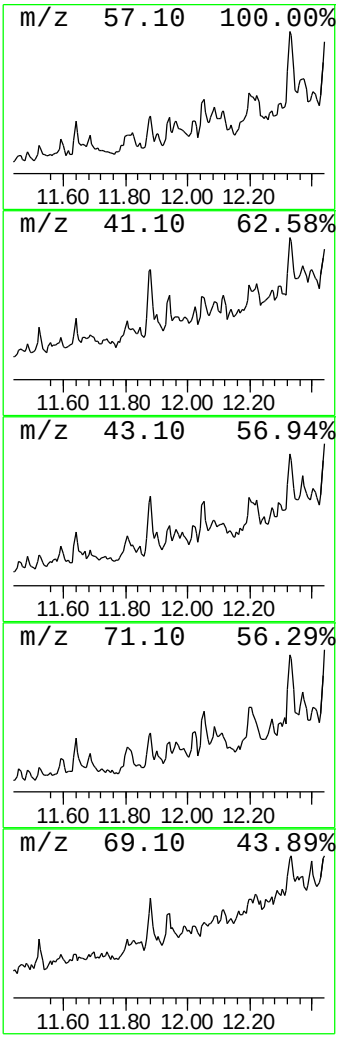
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Sulfurous acid, butyl octad... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	2.29 ng	101688	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	58
2	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	52
3	Tetracosane	338	C24H50	000646-31-1	46
4	Hexadecane	226	C16H34	000544-76-3	46
5	Octadecane	254	C18H38	000593-45-3	46





Library Search Compound Report

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Data File : BF112454.D
Acq On : 7 Feb 2019 22:32
Operator : JU/SJ
Sample : K1396-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 23935

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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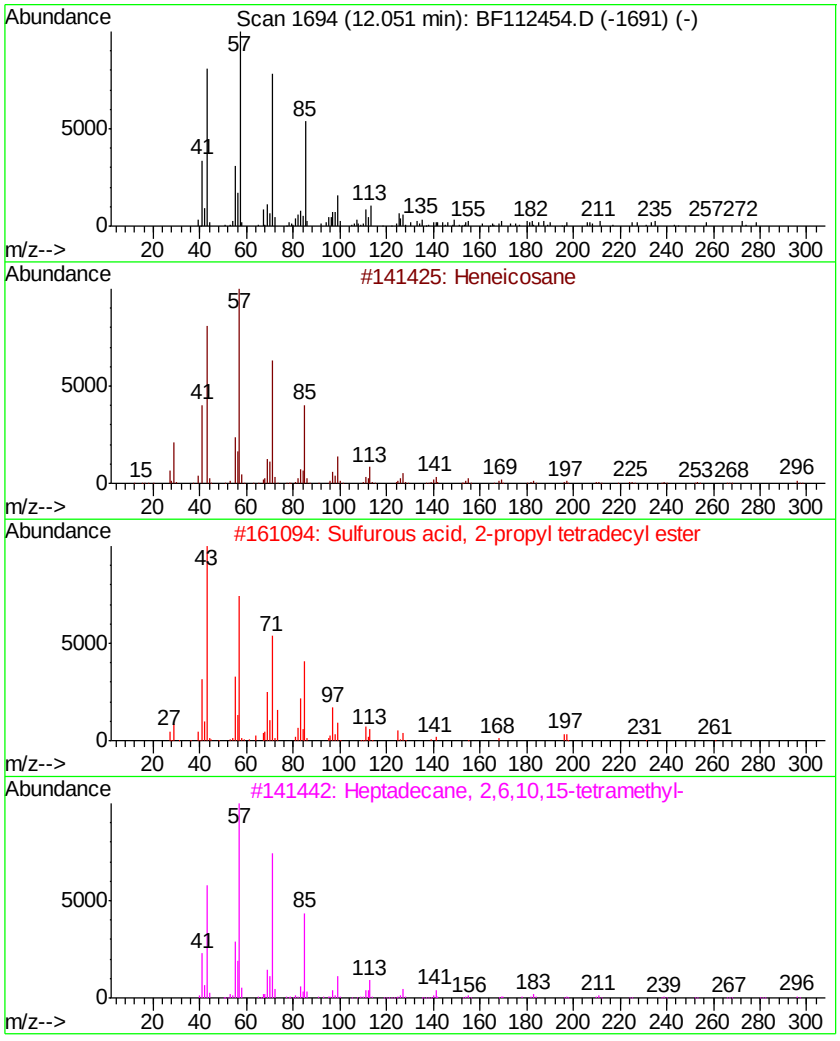
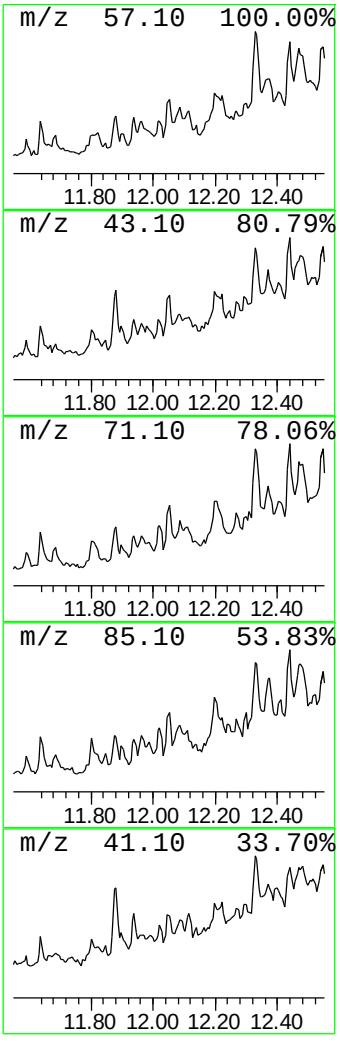
Peak Number 11 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	2.92 ng	129811	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	86
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
4	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	86
5	Heptadecane	240	C17H36	000629-78-7	86





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Sample : K1396-01
Misc :
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Instrument : BNA_F
ClientSampleId : 23935

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
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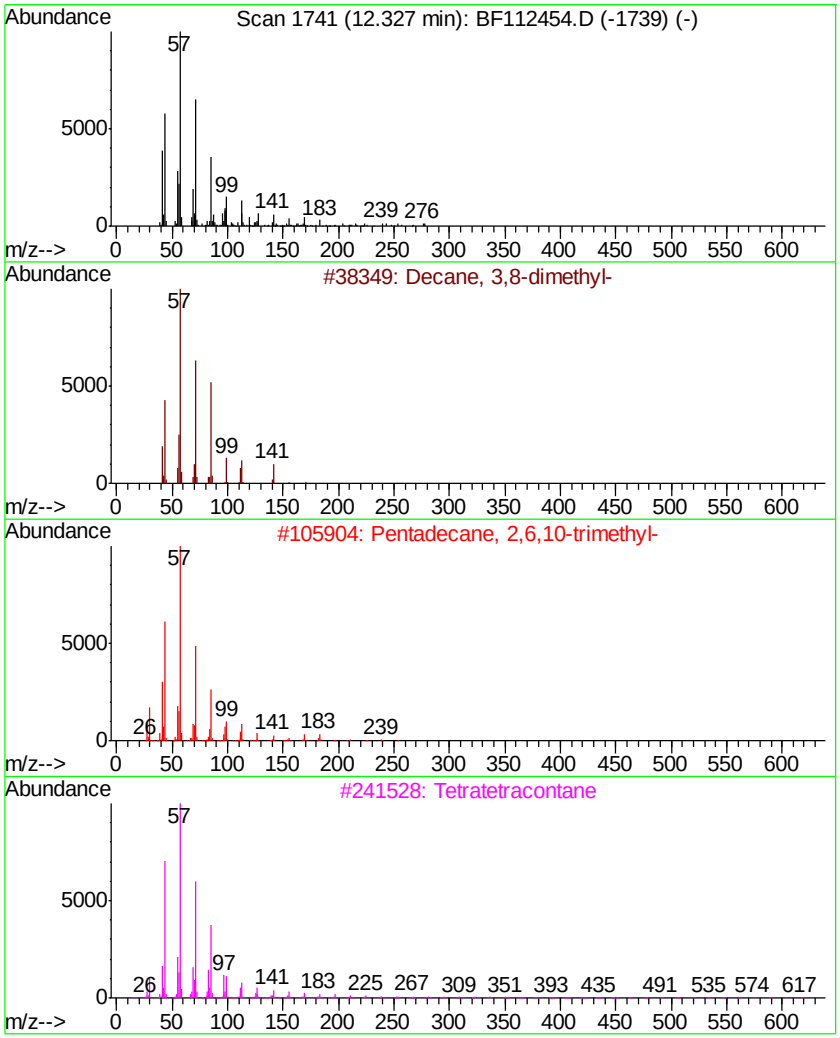
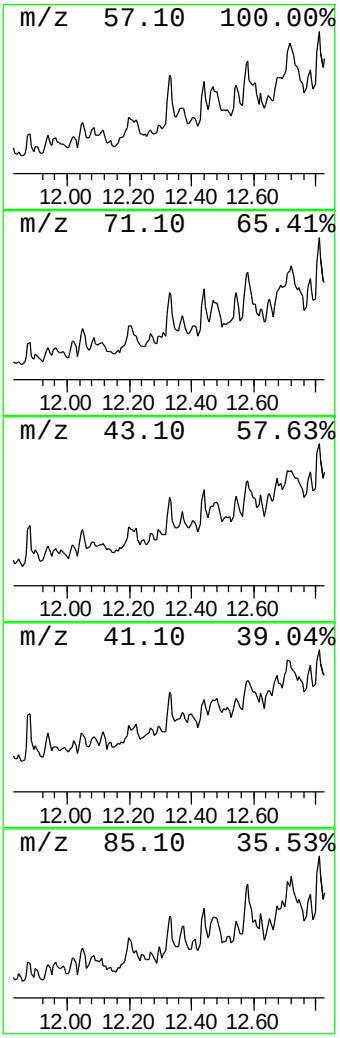
Peak Number 12 Decane, 3,8-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.33	4.65 ng	206793	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
3	Tetratetracontane	619	C44H90	007098-22-8	86
4	Heptadecane	240	C17H36	000629-78-7	83
5	Octadecane	254	C18H38	000593-45-3	83





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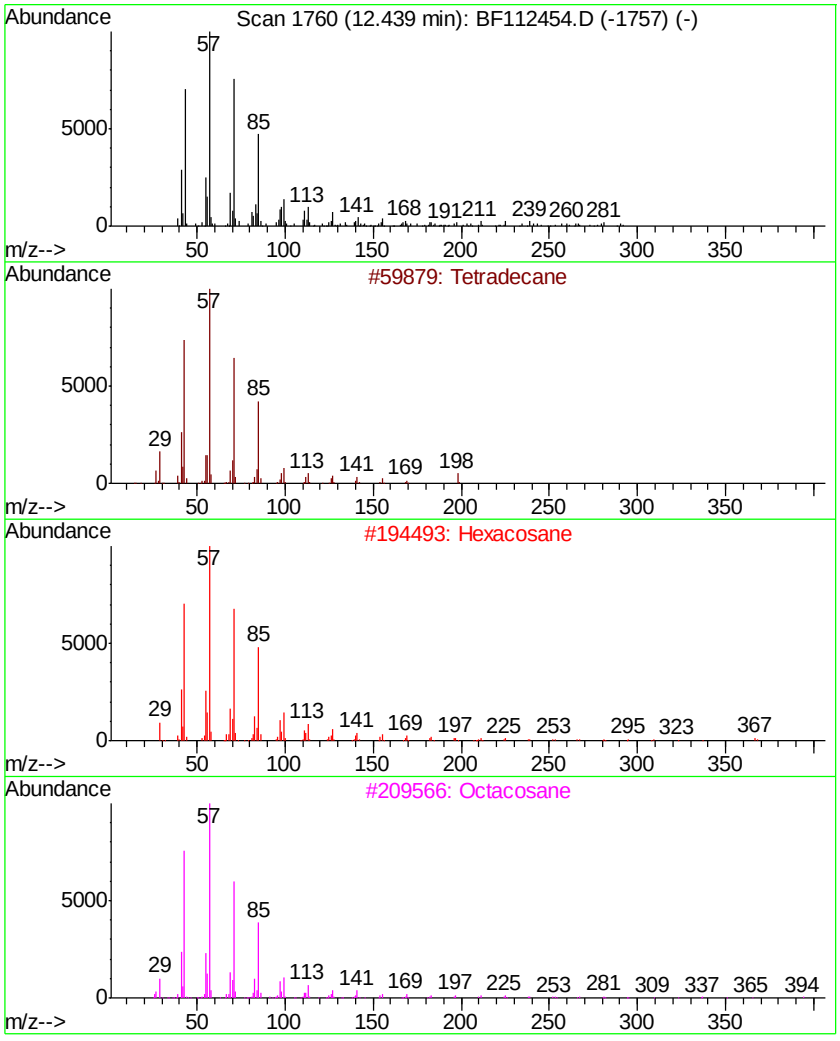
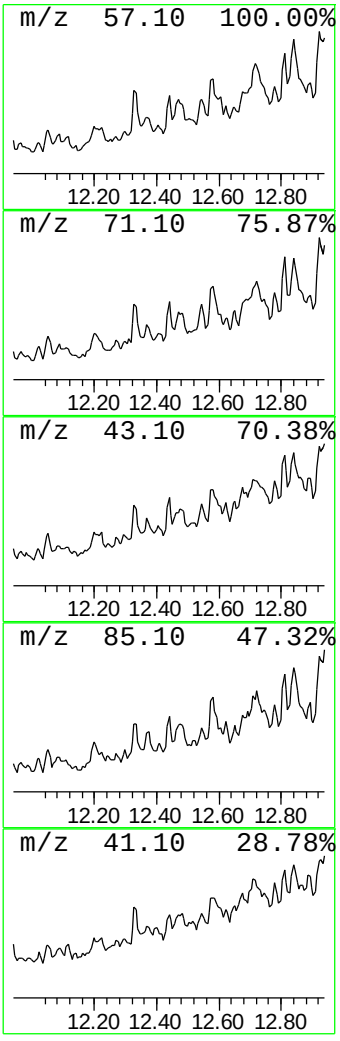
Peak Number 13 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	5.09 ng	226576	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Nonadecane	268	C19H40	000629-92-5	90





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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 23935

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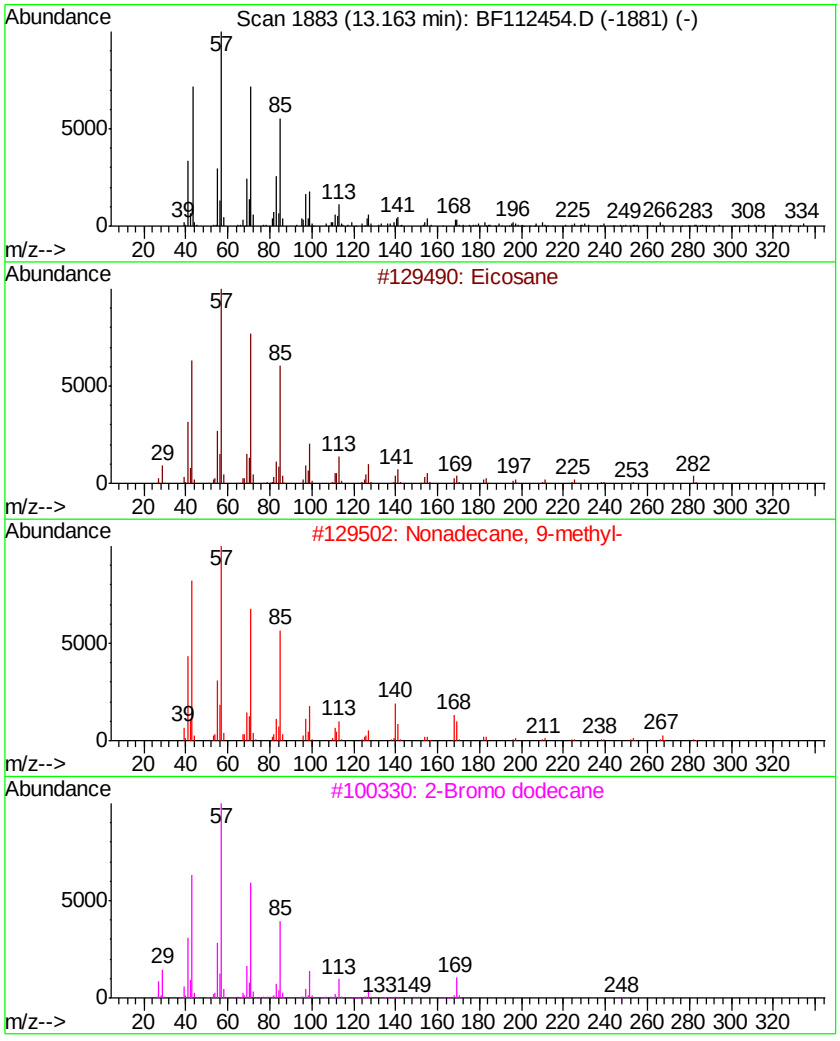
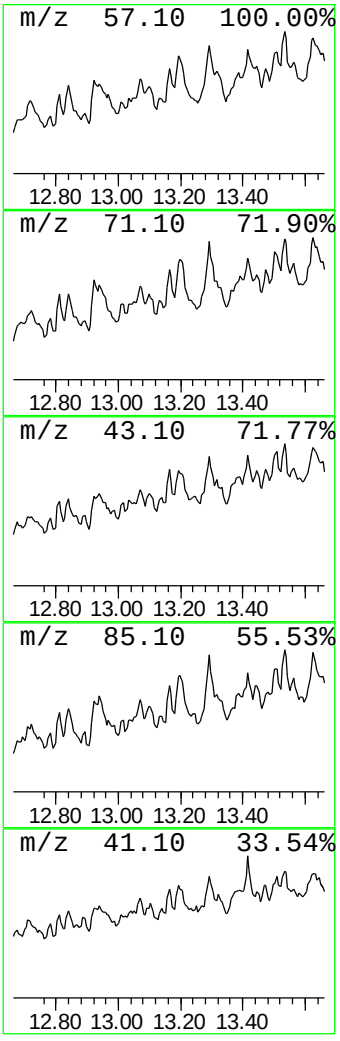
Peak Number 14 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.16	10.17 ng	252872	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	91
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
4	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	90
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	90





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Misc :
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Instrument : BNA_F
ClientSampleId : 23935

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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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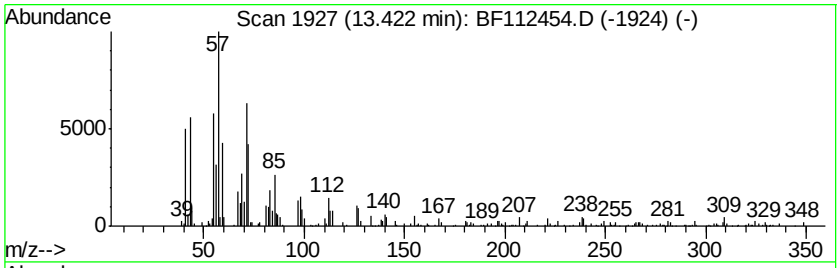
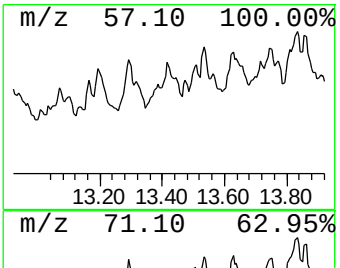
Peak Number 15 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	11.06 ng	274817	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	1-Chloroeicosane	316	C20H41Cl	042217-02-7	47
3	Tridecane	184	C13H28	000629-50-5	38
4	Hexadecane	226	C16H34	000544-76-3	38
5	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	38





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-methoxy...	2.12	3.0	ng	113225	1	6.83	755201	20.0
2-Pentanone, 4-hy...	5.06	2.9	ng	110150	1	6.83	755201	20.0
unknown6.61	6.61	69.4	ng	2621920	1	6.83	755201	20.0
1-Hexanol, 2-ethyl-	6.90	3.7	ng	140976	1	6.83	755201	20.0
Heptacosane	10.76	2.6	ng	115200	4	11.36	889621	20.0
Dodecane	11.25	2.8	ng	125068	4	11.36	889621	20.0
n-Hexadecanoic acid	11.88	5.0	ng	222425	4	11.36	889621	20.0
Sulfurous acid, b...	11.94	2.3	ng	101688	4	11.36	889621	20.0
Heneicosane	12.05	2.9	ng	129811	4	11.36	889621	20.0
Decane, 3,8-dimet...	12.33	4.7	ng	206793	4	11.36	889621	20.0
Tetradecane	12.44	5.1	ng	226576	4	11.36	889621	20.0
Eicosane	13.16	10.2	ng	252872	5	14.01	497145	20.0
9-Octadecenamide,...	13.42	11.1	ng	274817	5	14.01	497145	20.0