

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF101217\
 Data File : BF099411.D
 Acq On : 12 Oct 2017 22:52
 Operator : SJ/JU
 Sample : I5729-11
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 6W-(2-3)

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.134	6	8	36	rVB4	90099	310176	14.74%	1.451%
2	5.075	505	508	522	rBV	255012	331238	15.74%	1.549%
3	5.475	572	576	591	rBV	1860386	1920526	91.28%	8.983%
4	6.486	743	748	751	rBV	1963116	1913184	90.94%	8.948%
5	6.622	767	771	775	rBV	2186816	2001512	95.13%	9.362%
6	6.851	806	810	816	rBV	799620	639229	30.38%	2.990%
7	7.010	833	837	840	rBV	1775893	1586260	75.40%	7.419%
8	7.416	901	906	909	rBV	1310265	1204693	57.26%	5.635%
9	8.133	1024	1028	1031	rBV	1036755	828025	39.36%	3.873%
10	9.204	1205	1210	1214	rBV	2279383	2103886	100.00%	9.840%
11	9.598	1274	1277	1285	rVB	269365	213180	10.13%	0.997%
12	9.751	1299	1303	1308	rBV	123358	108106	5.14%	0.506%
13	9.810	1308	1313	1318	rBV2	19506	23438	1.11%	0.110%
14	9.886	1322	1326	1330	rBV	943196	811933	38.59%	3.798%
15	10.304	1394	1397	1401	rVB	32096	26027	1.24%	0.122%
16	10.598	1441	1447	1449	rBV2	29000	29305	1.39%	0.137%
17	10.674	1456	1460	1471	rVB	978998	918456	43.66%	4.296%
18	10.780	1475	1478	1487	rVB2	37468	57800	2.75%	0.270%
19	11.227	1550	1554	1556	rBV2	28898	24965	1.19%	0.117%
20	11.374	1575	1579	1581	rBV	824678	676063	32.13%	3.162%
21	11.398	1581	1583	1588	rVV	236219	184123	8.75%	0.861%
22	11.451	1588	1592	1595	rVB	112263	91468	4.35%	0.428%
23	11.610	1614	1619	1622	rBV2	23166	27927	1.33%	0.131%
24	11.874	1659	1664	1665	rBV	31196	26838	1.28%	0.126%
25	11.904	1666	1669	1674	rVB	42983	43764	2.08%	0.205%
26	11.951	1674	1677	1680	rBV	26506	22045	1.05%	0.103%
27	11.986	1680	1683	1686	rBV	45289	54797	2.60%	0.256%
28	12.421	1752	1757	1759	rBV	25092	27711	1.32%	0.130%
29	12.515	1769	1773	1777	rVB4	19879	23734	1.13%	0.111%
30	12.586	1782	1785	1789	rBV	339879	285636	13.58%	1.336%
31	12.680	1798	1801	1805	rBV	41286	39268	1.87%	0.184%
32	12.815	1818	1824	1827	rBV	293028	301532	14.33%	1.410%
33	12.957	1843	1848	1851	rBV	1549062	1413335	67.18%	6.611%
34	13.033	1857	1861	1865	rBV3	21400	36672	1.74%	0.172%

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35	13.145	1872	1880	1883	rBV	48723	71744	3.41%	0.336%
36	13.210	1888	1891	1893	rVV	39134	30427	1.45%	0.142%
37	13.245	1893	1897	1900	rVV2	28082	33476	1.59%	0.157%
38	13.657	1964	1967	1970	rVB	28437	26229	1.25%	0.123%
39	13.762	1982	1985	1987	rBV2	30071	25424	1.21%	0.119%
40	13.839	1995	1998	2000	rBV3	64707	64597	3.07%	0.302%
41	13.862	2000	2002	2005	rVB	35163	30097	1.43%	0.141%
42	14.015	2023	2028	2031	rBV2	785587	844855	40.16%	3.952%
43	14.039	2031	2032	2038	rVB	153712	109607	5.21%	0.513%
44	14.162	2051	2053	2059	rBV5	20716	23671	1.13%	0.111%
45	14.398	2091	2093	2096	rVB2	41841	35493	1.69%	0.166%
46	14.545	2116	2118	2123	rVB6	26388	22934	1.09%	0.107%
47	14.751	2150	2153	2158	rBV2	74397	85432	4.06%	0.400%
48	15.056	2201	2205	2208	rBV	140949	205522	9.77%	0.961%
49	15.162	2220	2223	2229	rBV	61402	82579	3.93%	0.386%
50	15.362	2253	2257	2262	rVB	106624	154106	7.32%	0.721%
51	15.421	2263	2267	2272	rBV	138605	164898	7.84%	0.771%
52	15.486	2273	2278	2282	rBV	421600	556884	26.47%	2.605%
53	15.909	2346	2350	2355	rVB3	52040	68657	3.26%	0.321%
54	16.409	2430	2435	2440	rVB3	55903	92444	4.39%	0.432%
55	16.962	2525	2529	2541	rVB2	69178	198558	9.44%	0.929%
56	17.409	2601	2605	2616	rVB	69102	145536	6.92%	0.681%

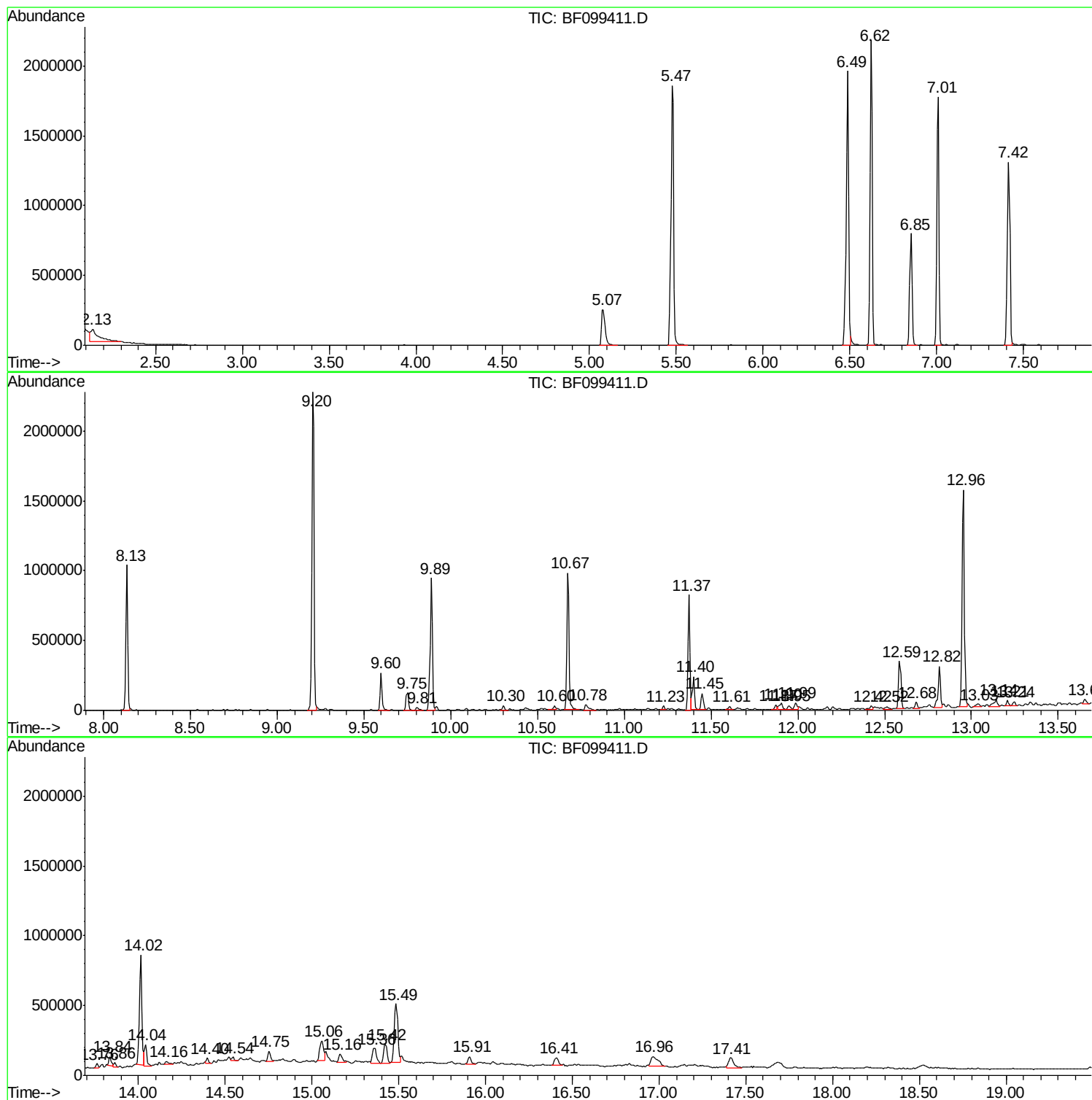
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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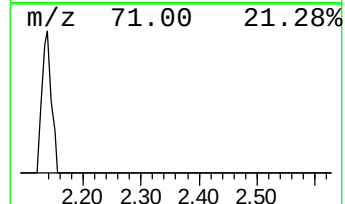
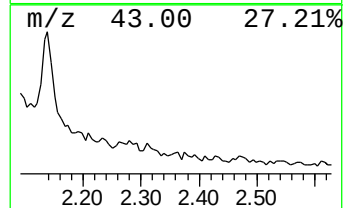
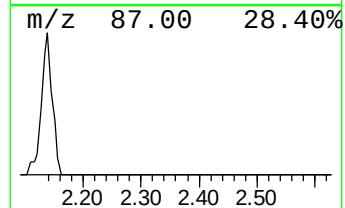
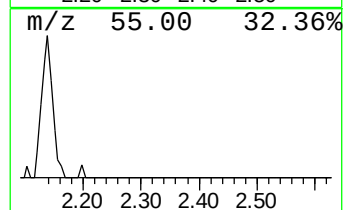
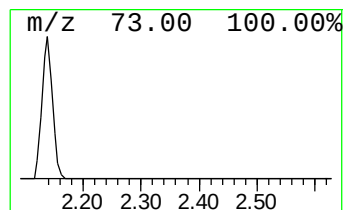
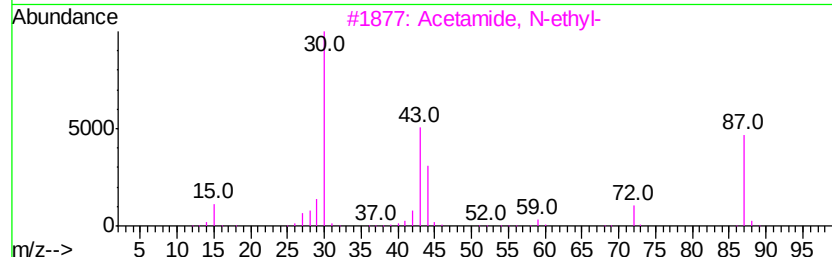
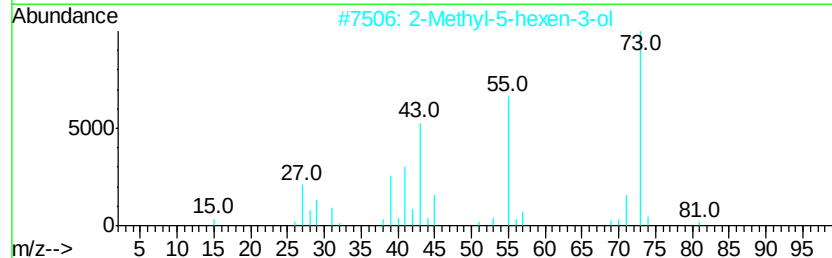
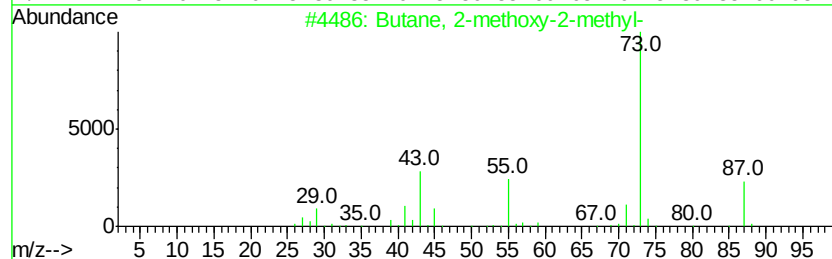
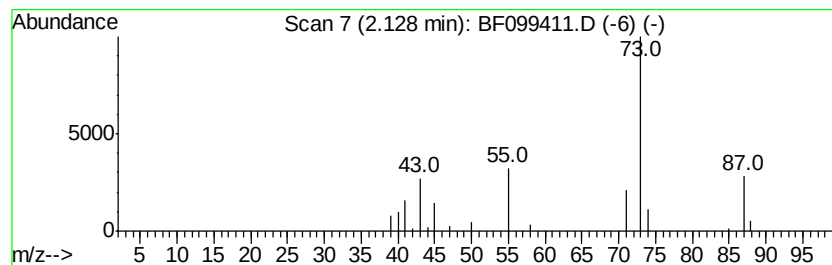
Instrument :
BNA_F
ClientSampleId :
6W-(2-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.13	9.70 ng	310176	1,4-Dichlorobenzene-d4	6.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	33
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
5	Isobutylamine	73	C4H11N	000078-81-9	5



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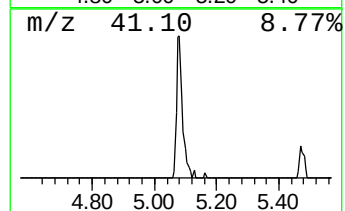
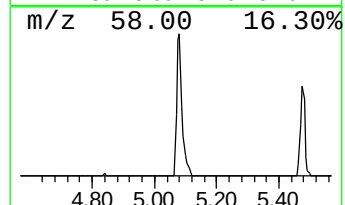
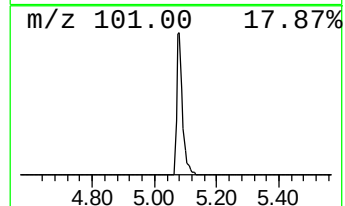
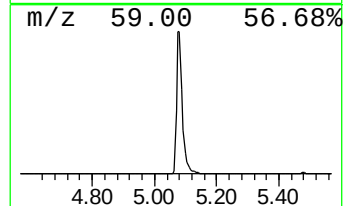
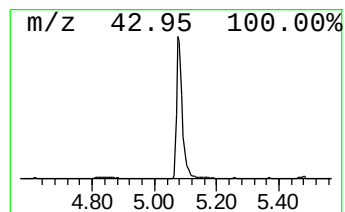
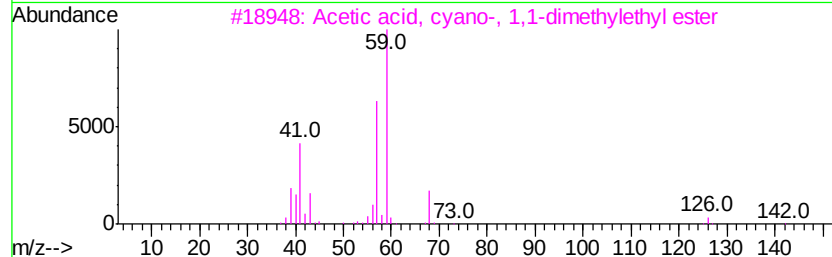
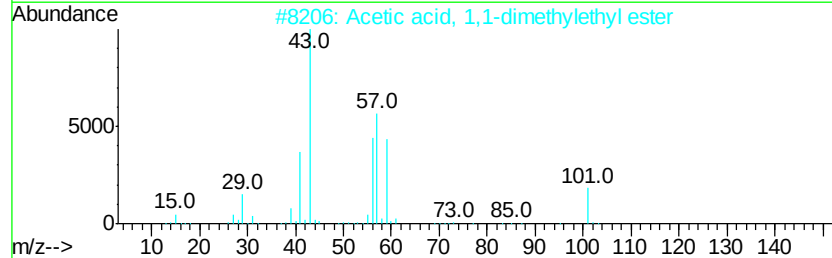
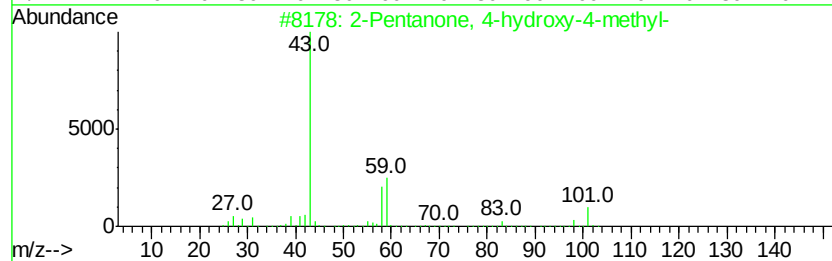
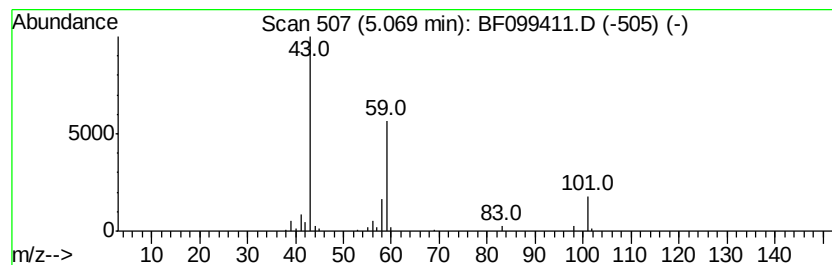
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	10.36 ng	331238	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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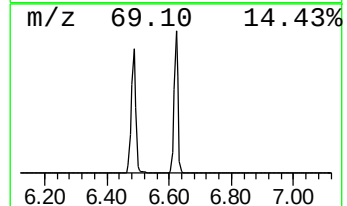
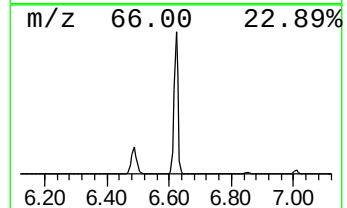
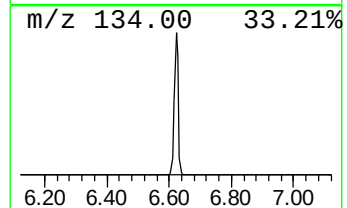
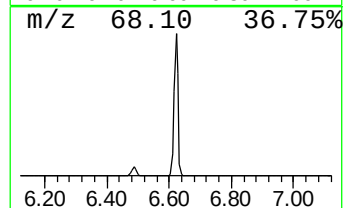
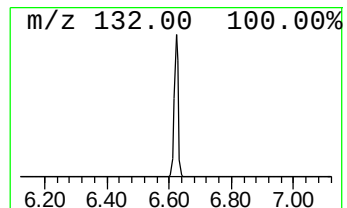
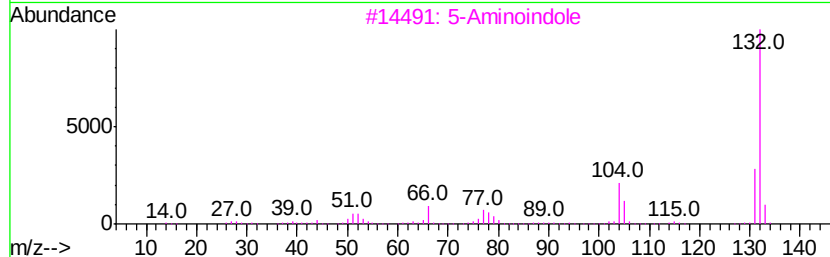
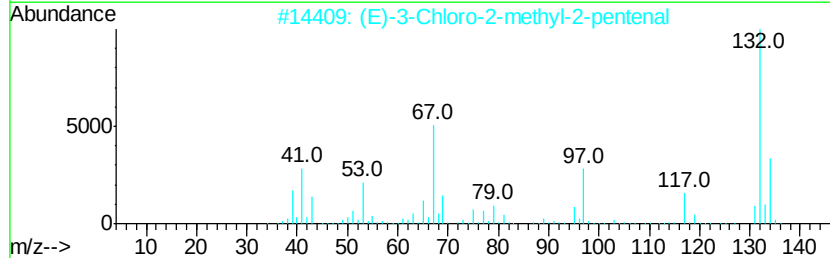
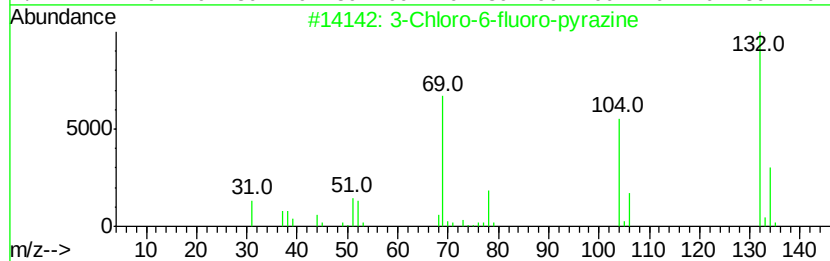
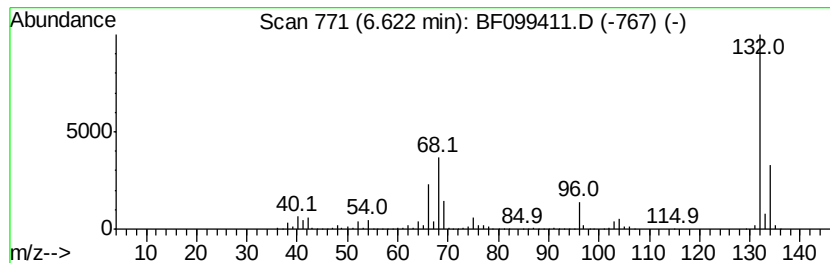
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	62.62 ng	2001510	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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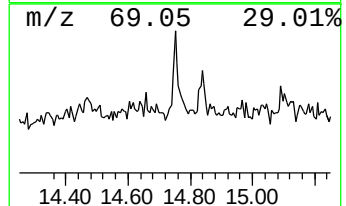
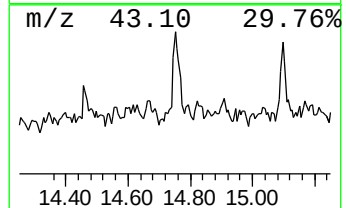
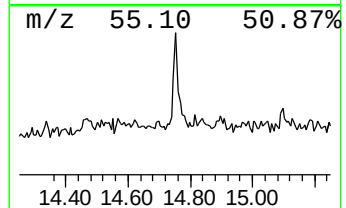
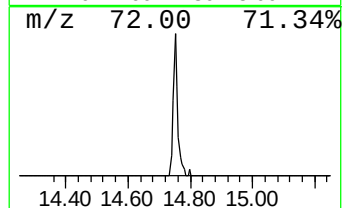
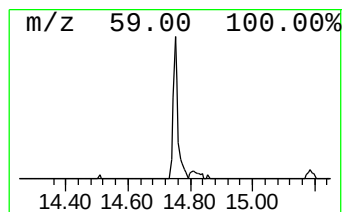
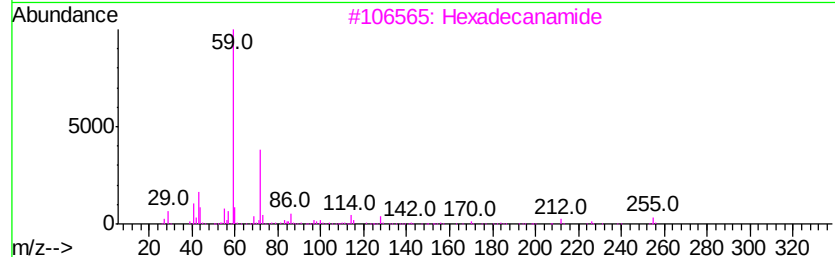
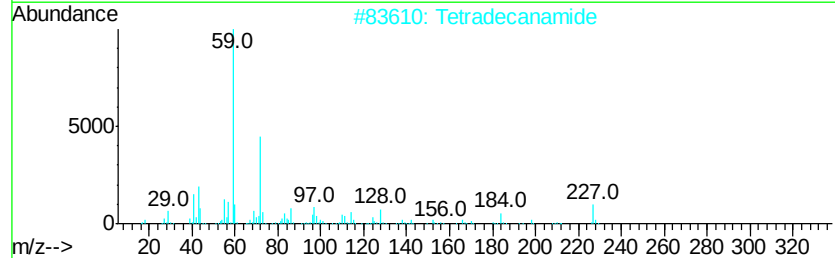
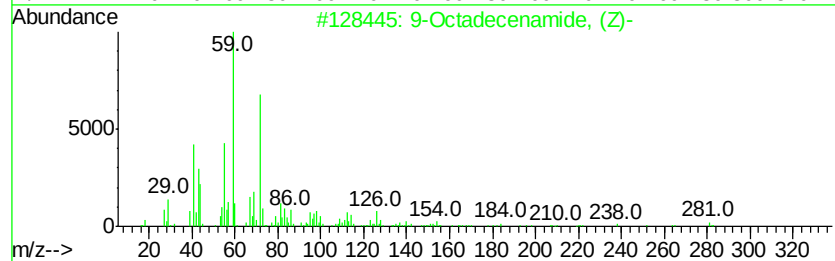
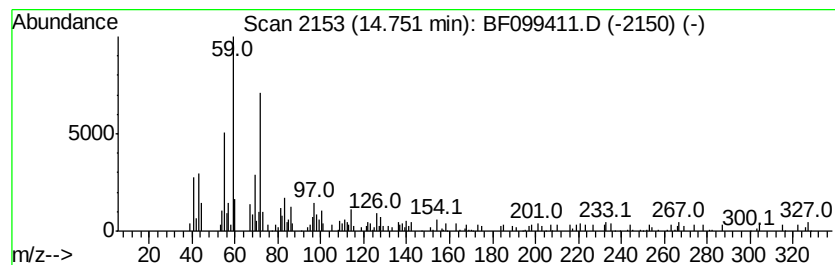
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	3.07 ng	85432	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	89
2		Tetradecanamide	227	C14H29NO	000638-58-4	59
3		Hexadecanamide	255	C16H33NO	000629-54-9	59
4		Octanamide	143	C8H17NO	000629-01-6	59
5		Octadecanamide	283	C18H37NO	000124-26-5	47



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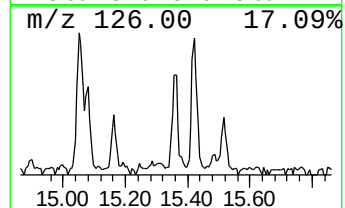
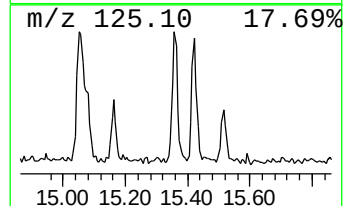
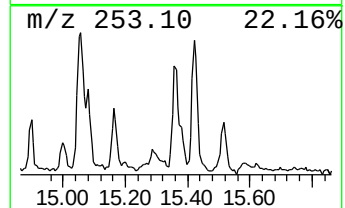
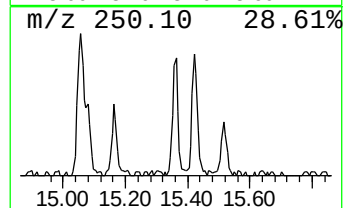
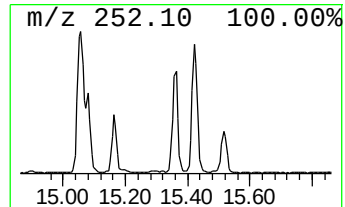
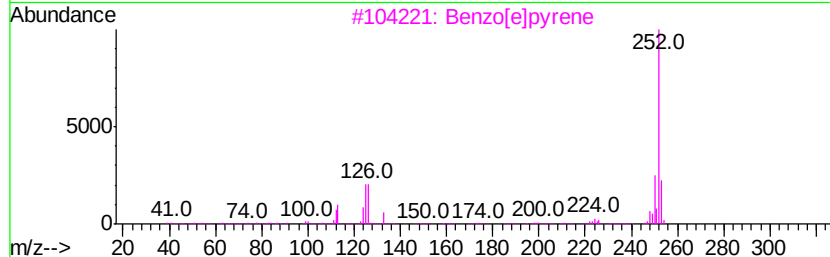
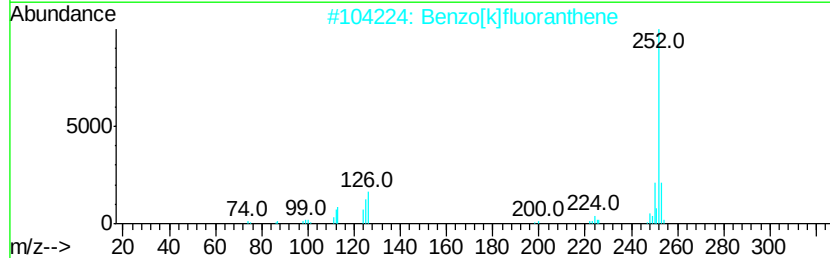
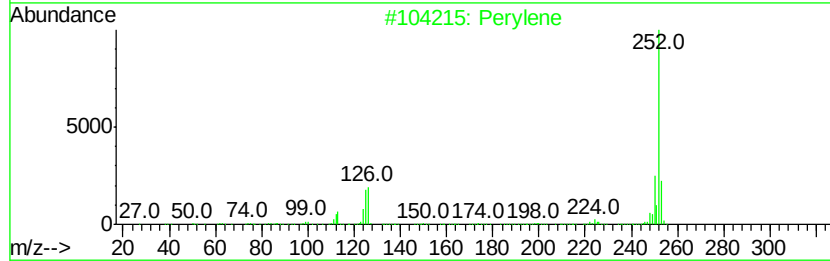
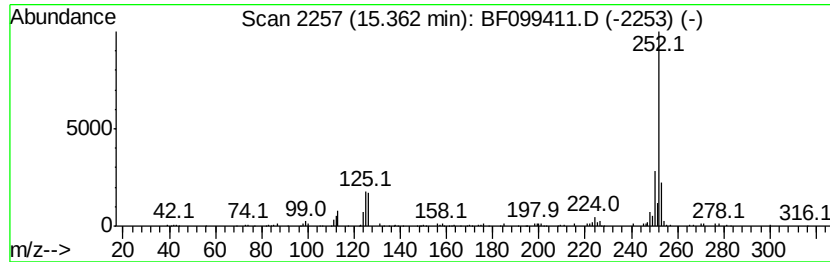
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	5.53 ng	154106	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Perylene	252	C20H12	000198-55-0	99
2		Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3		Benzo[e]pyrene	252	C20H12	000192-97-2	98
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	96
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	96



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF101217\
Data File : BF099411.D
Acq On : 12 Oct 2017 22:52
Operator : SJ/JU
Sample : I5729-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
6W-(2-3)

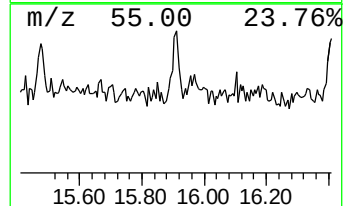
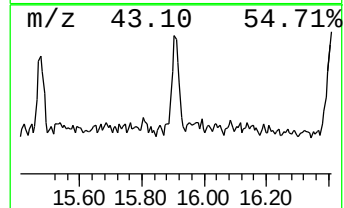
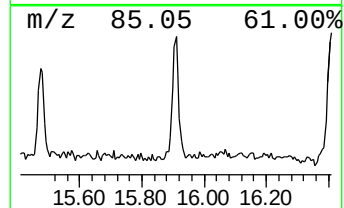
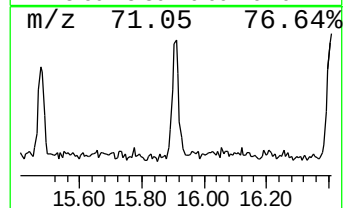
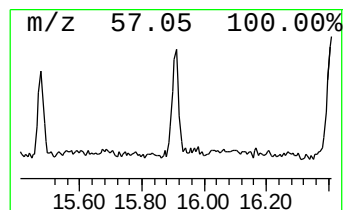
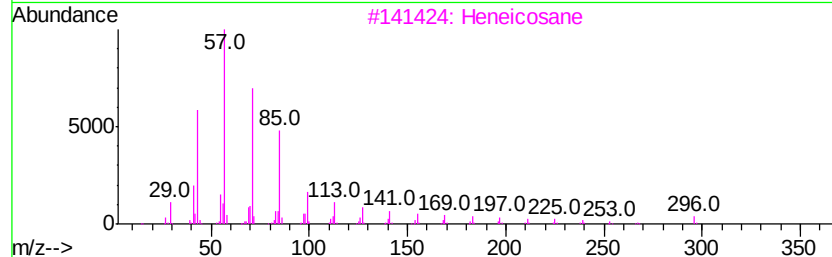
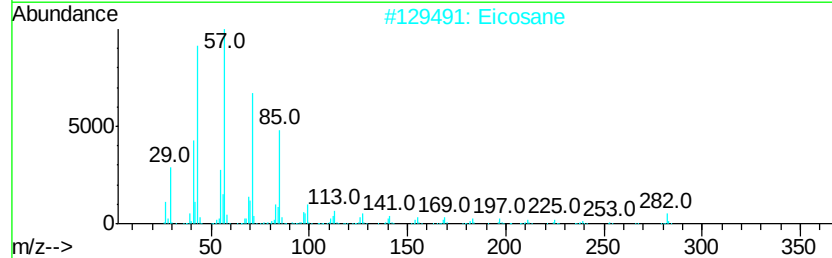
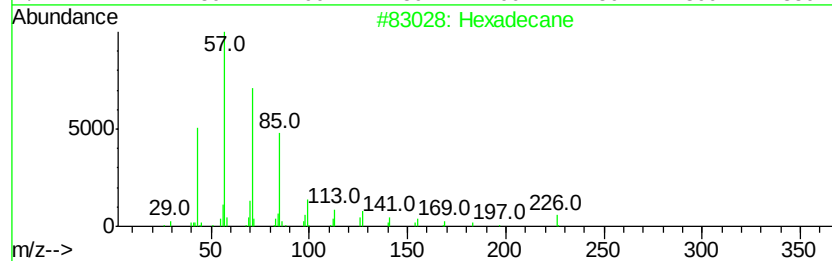
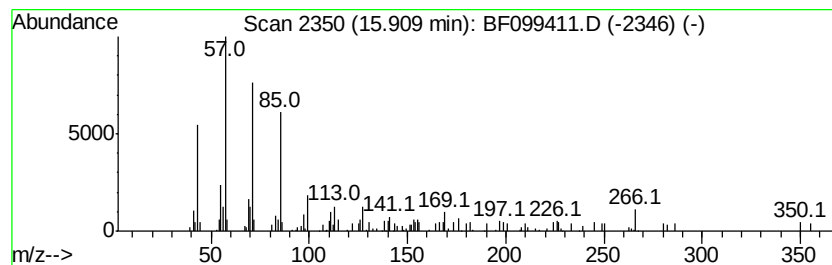
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	2.47 ng	68657	Perylene-d12	15.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	86
2	Eicosane		282	C20H42	000112-95-8	76
3	Heneicosane		296	C21H44	000629-94-7	62
4	Docosane		310	C22H46	000629-97-0	62
5	Octadecane		254	C18H38	000593-45-3	58



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF101217\
Data File : BF099411.D
Acq On : 12 Oct 2017 22:52
Operator : SJ/JU
Sample : I5729-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
6W-(2-3)

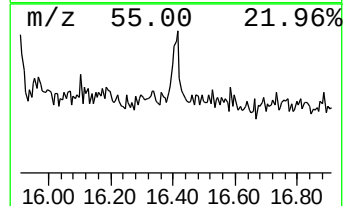
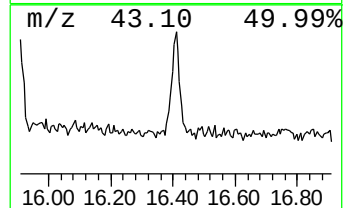
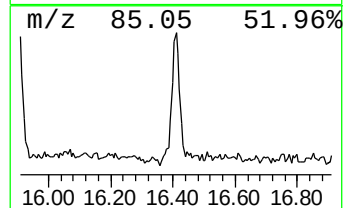
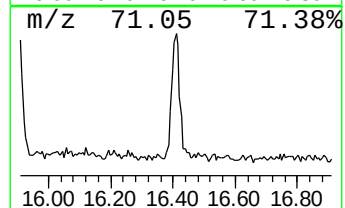
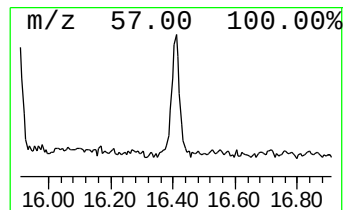
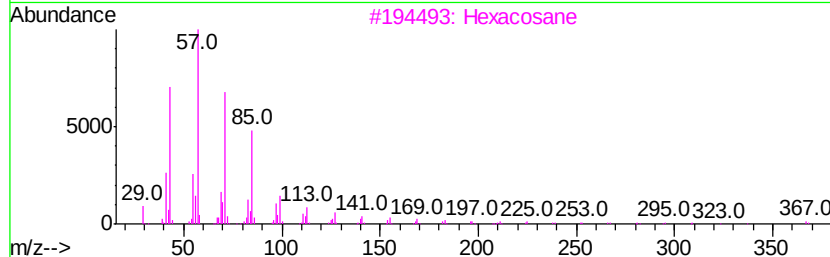
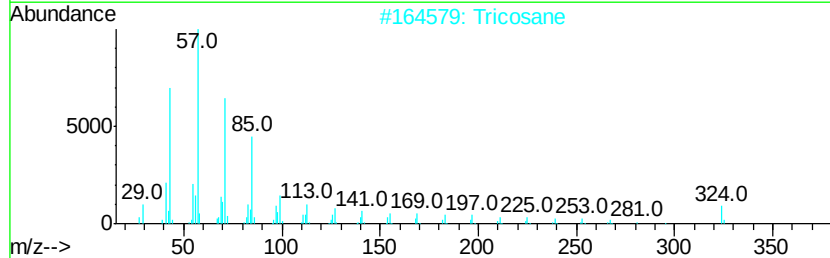
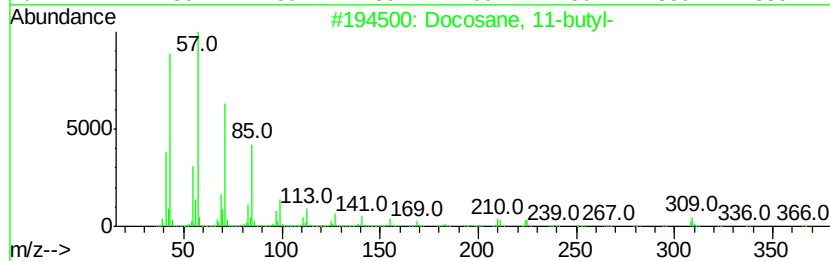
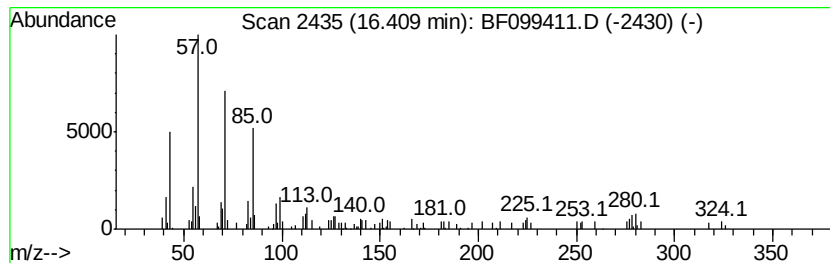
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosane, 11-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	3.32 ng	92444	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 11-butyl-	366	C26H54	013475-76-8	68
2		Tricosane	324	C23H48	000638-67-5	64
3		Hexacosane	366	C26H54	000630-01-3	62
4		Triacontane	422	C30H62	000638-68-6	62
5		2-methyloctacosane	408	C29H60	1000376-72-8	62



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF101217\
Data File : BF099411.D
Acq On : 12 Oct 2017 22:52
Operator : SJ/JU
Sample : I5729-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
6W-(2-3)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	9.7	ng	310176	1	6.85	639229	20.0
2-Pentanone, 4-hy...	5.07	10.4	ng	331238	1	6.85	639229	20.0
unknown6.62	6.62	62.6	ng	2001510	1	6.85	639229	20.0
9-Octadecenamide, ...	14.75	3.1	ng	85432	6	15.49	556884	20.0
Perylene	15.36	5.5	ng	154106	6	15.49	556884	20.0
Hexadecane	15.91	2.5	ng	68657	6	15.49	556884	20.0
Docosane, 11-butyl-	16.41	3.3	ng	92444	6	15.49	556884	20.0