

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
 Data File : BF097103.D
 Acq On : 27 Jul 2017 4:10
 Operator : SJ/JU
 Sample : I4415-01
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-02-072417

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-BF072517.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	2.646	127	129	145	rBV	21195	88419	3.72%	0.467%
2	4.634	463	467	479	rBV	154760	234879	9.88%	1.241%
3	5.092	540	545	559	rBV	2161144	2378261	100.00%	12.561%
4	6.157	722	726	741	rBV	1985024	2266008	95.28%	11.968%
5	6.269	741	745	748	rBV	2348862	2068357	86.97%	10.925%
6	6.492	780	783	791	rBV	590905	562374	23.65%	2.970%
7	6.651	806	810	821	rBV	1699247	1485974	62.48%	7.849%
8	7.063	876	880	883	rBV	1403742	1222893	51.42%	6.459%
9	7.780	998	1002	1006	rBV	826237	705520	29.67%	3.726%
10	8.857	1181	1185	1188	rBV	2107454	1801485	75.75%	9.515%
11	9.257	1250	1253	1255	rBV	210097	150078	6.31%	0.793%
12	9.480	1288	1291	1295	rBV	26062	25859	1.09%	0.137%
13	9.527	1295	1299	1302	rVB	633001	591153	24.86%	3.122%
14	9.757	1337	1338	1344	rVB3	24680	27831	1.17%	0.147%
15	9.980	1373	1376	1380	rVB	72420	55866	2.35%	0.295%
16	10.198	1409	1413	1416	rBV	35170	42501	1.79%	0.224%
17	10.310	1429	1432	1438	rBV	1123729	1008330	42.40%	5.326%
18	10.451	1453	1456	1457	rBV	66314	58091	2.44%	0.307%
19	10.898	1529	1532	1534	rBV	45847	34004	1.43%	0.180%
20	10.927	1534	1537	1543	rVB	35468	37210	1.56%	0.197%
21	10.998	1545	1549	1552	rBV	605876	528526	22.22%	2.792%
22	11.021	1552	1553	1557	rVB	61859	38078	1.60%	0.201%
23	11.074	1560	1562	1565	rBV	44520	42218	1.78%	0.223%
24	11.321	1601	1604	1609	rBV2	33127	34503	1.45%	0.182%
25	11.504	1632	1635	1637	rBV2	35169	40178	1.69%	0.212%
26	11.557	1642	1644	1646	rVV	87253	67281	2.83%	0.355%
27	11.610	1650	1653	1656	rBV	52745	53422	2.25%	0.282%
28	11.727	1671	1673	1677	rBV2	24600	27922	1.17%	0.147%
29	12.051	1725	1728	1731	rBV	45024	71215	2.99%	0.376%
30	12.204	1751	1754	1759	rBV	191299	193140	8.12%	1.020%
31	12.257	1761	1763	1767	rVB4	30118	32081	1.35%	0.169%
32	12.339	1774	1777	1784	rBV6	69475	115827	4.87%	0.612%
33	12.427	1788	1792	1796	rBV	242425	278823	11.72%	1.473%
34	12.586	1815	1819	1822	rBV	1396689	1294794	54.44%	6.839%

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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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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35	12.762	1847	1849	1852	rVB2	47388	40199	1.69%	0.212%
36	12.827	1858	1860	1864	rVB2	41193	43334	1.82%	0.229%
37	12.863	1864	1866	1869	rBV	35617	35993	1.51%	0.190%
38	13.021	1891	1893	1898	rVB4	51241	45283	1.90%	0.239%
39	13.180	1918	1920	1923	rBV3	47504	49933	2.10%	0.264%
40	13.404	1956	1958	1959	rBV2	62054	58819	2.47%	0.311%
41	13.504	1972	1975	1981	rVB3	115642	155421	6.54%	0.821%
42	13.627	1992	1996	1999	rBV	512957	554466	23.31%	2.929%
43	14.980	2224	2226	2229	rBV	191174	195972	8.24%	1.035%
44	19.150	2931	2935	2936	rBV4	55669	90609	3.81%	0.479%

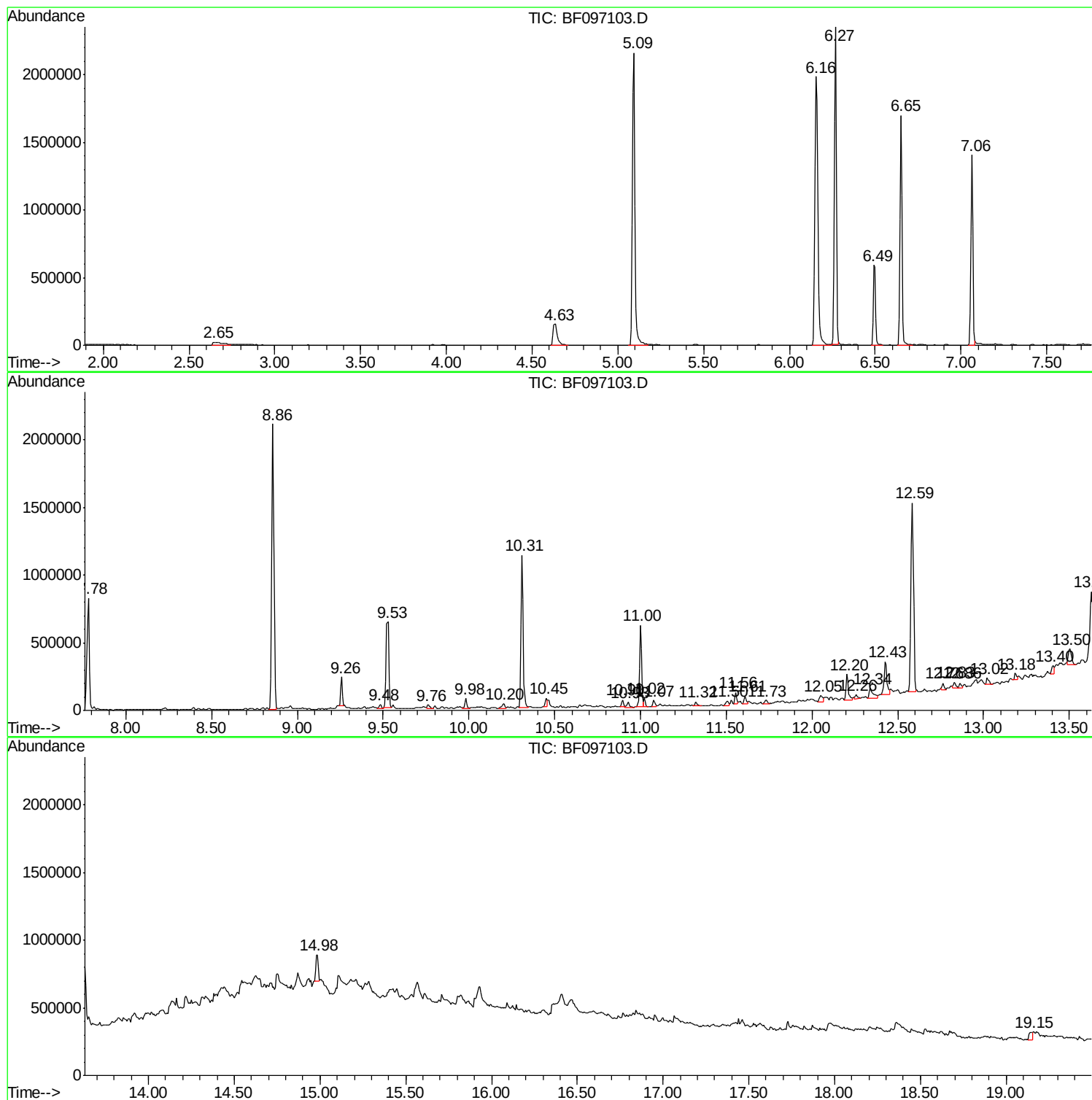
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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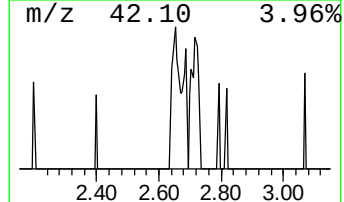
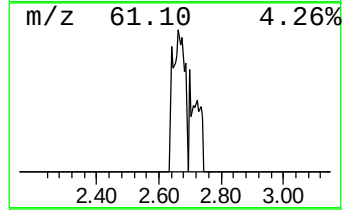
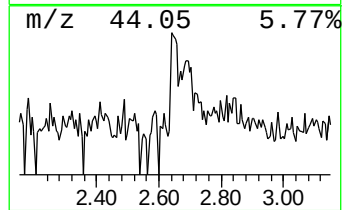
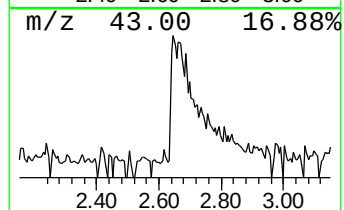
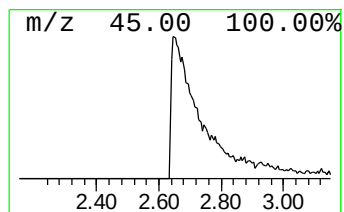
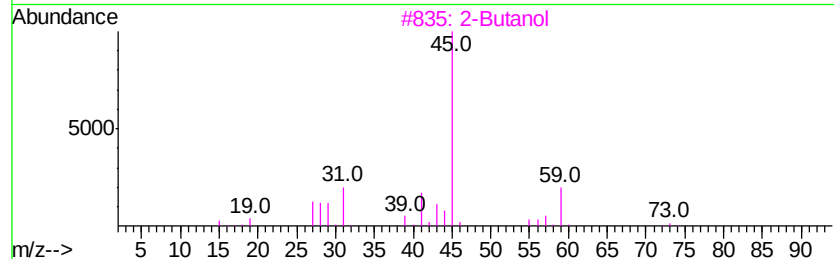
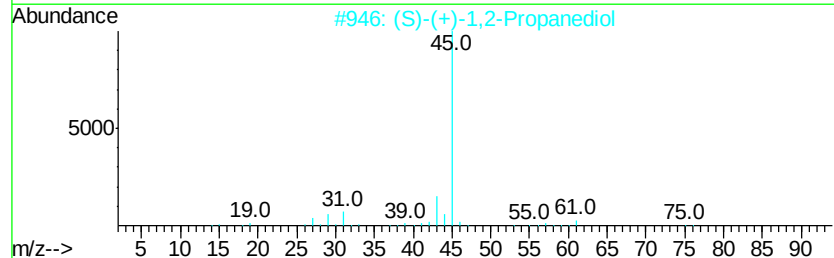
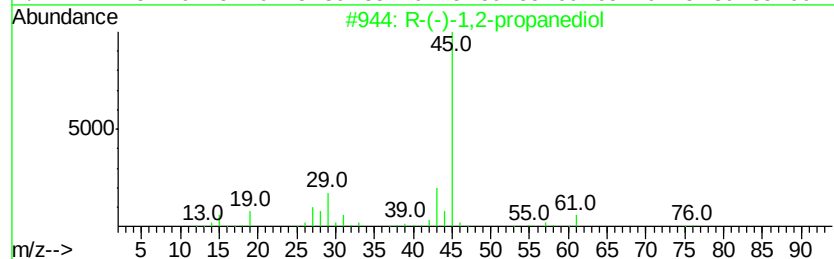
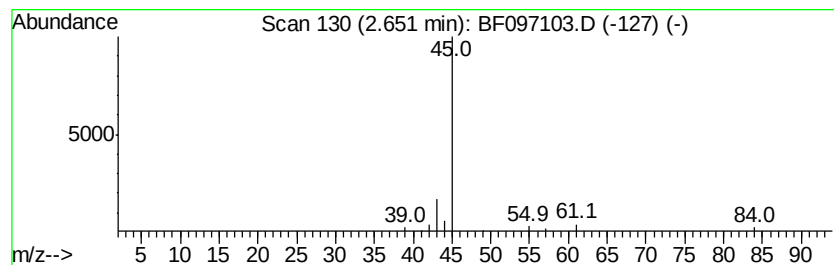
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.65 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.65	3.14 ng	88419	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3		2-Butanol	74	C4H10O	000078-92-2	9
4		2-Hexanol	102	C6H14O	000626-93-7	9
5		Propylene Glycol	76	C3H8O2	000057-55-6	9



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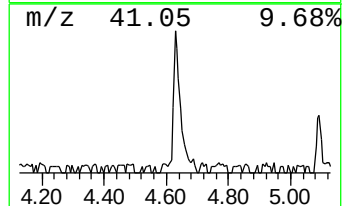
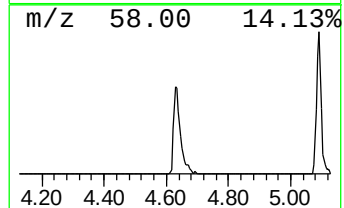
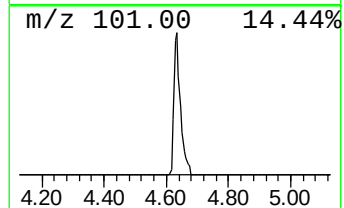
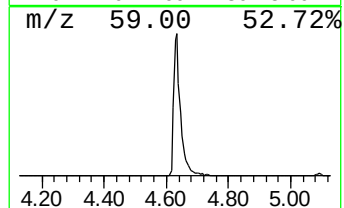
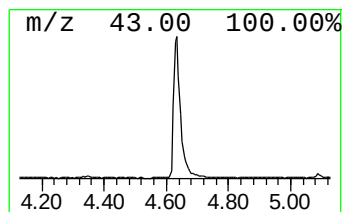
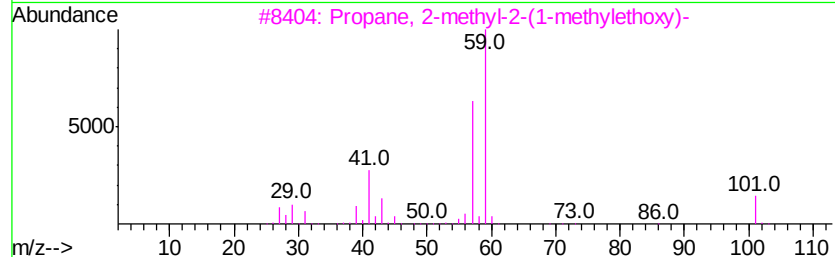
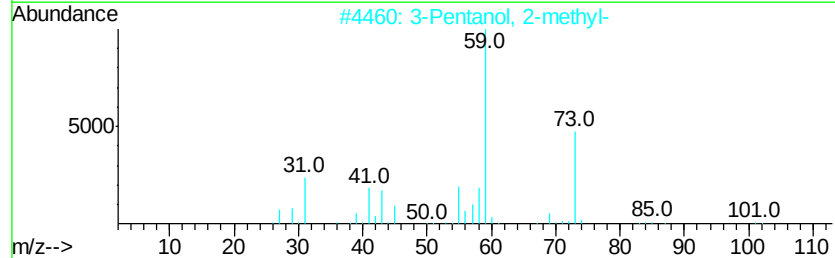
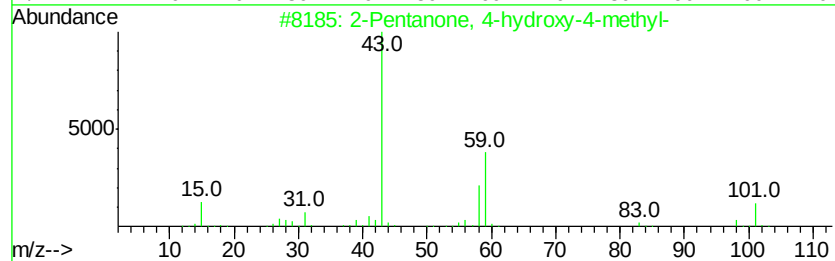
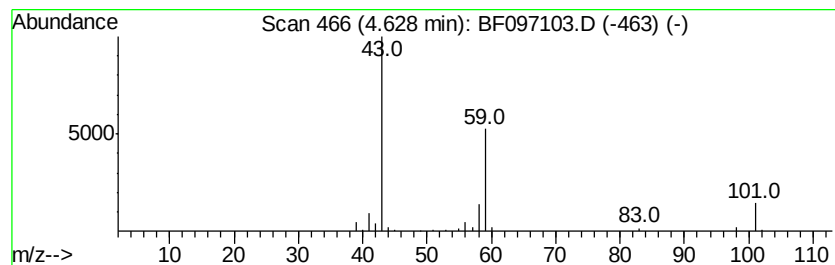
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.63	8.35 ng	234879	1,4-Dichlorobenzene-d4	6.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	47
3			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	42
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Butane	58	C4H10	000106-97-8	9



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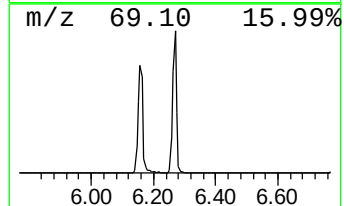
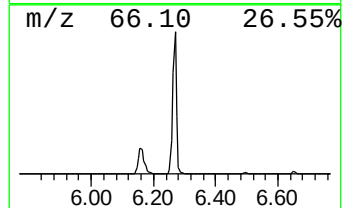
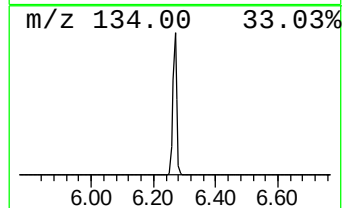
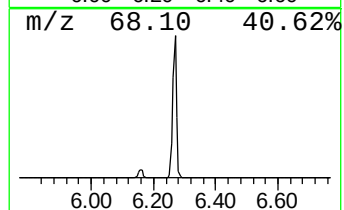
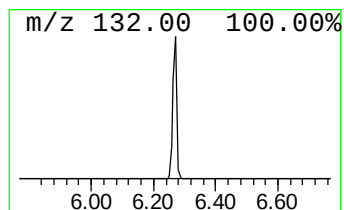
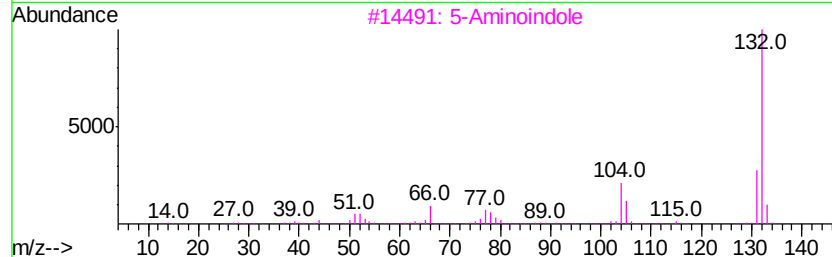
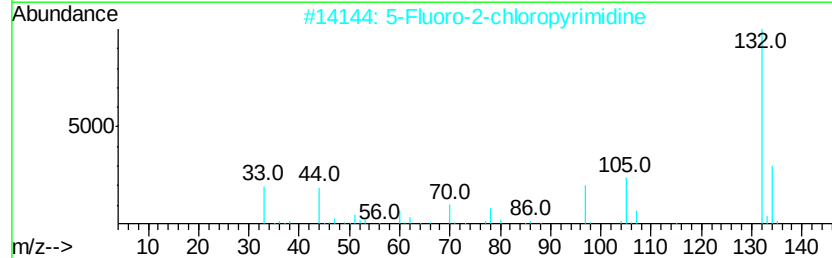
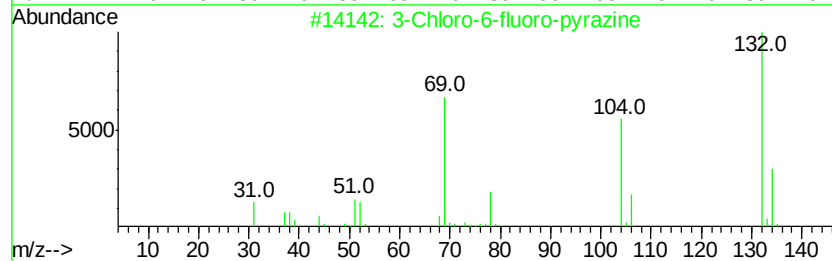
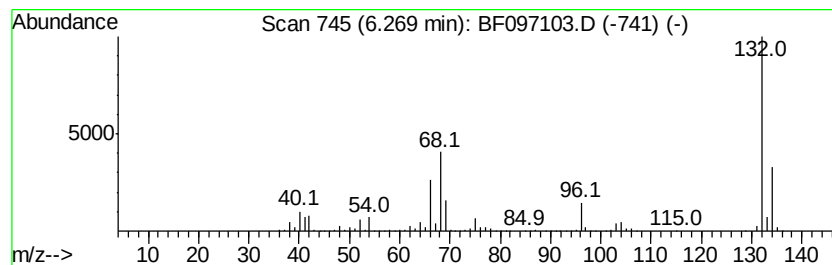
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	73.56 ng	2068360	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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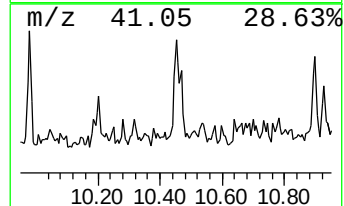
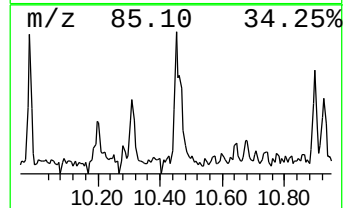
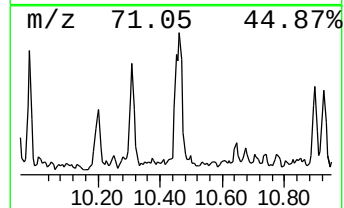
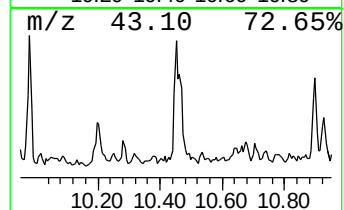
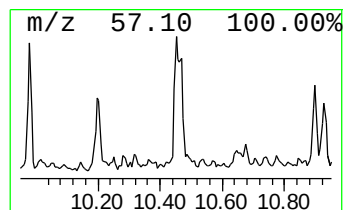
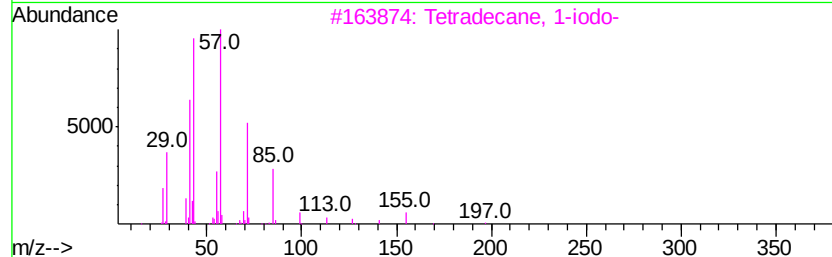
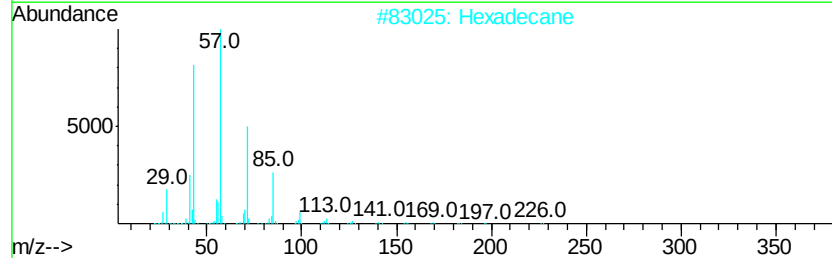
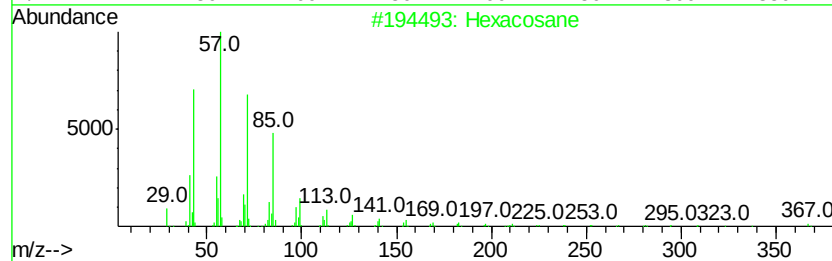
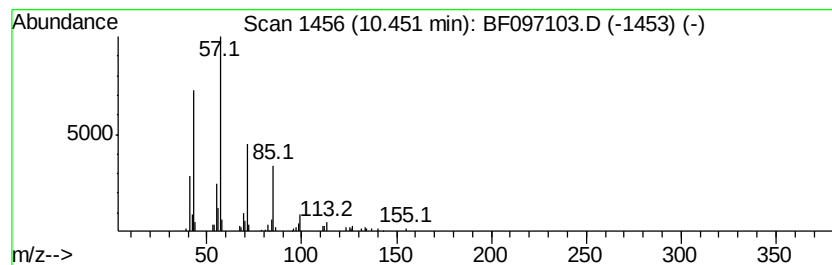
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.45	2.20 ng	58091	Phenanthrene-d10		11.00
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	86
2	Hexadecane	226	C16H34	000544-76-3	83
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80
5	Eicosane	282	C20H42	000112-95-8	72



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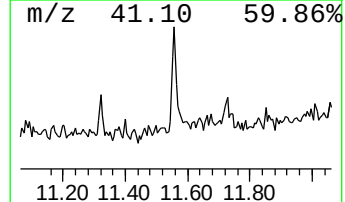
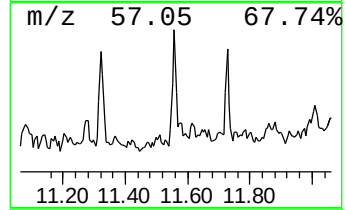
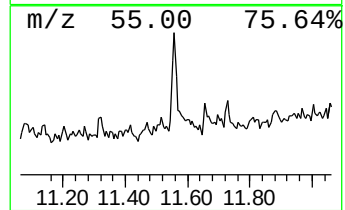
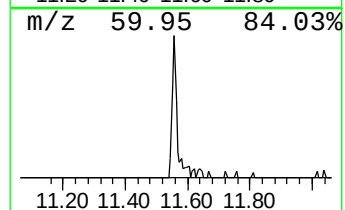
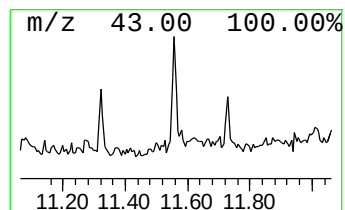
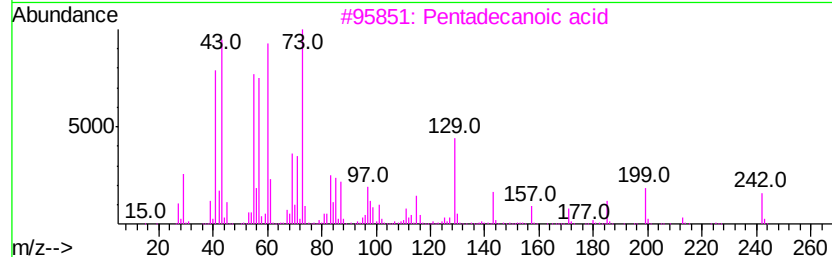
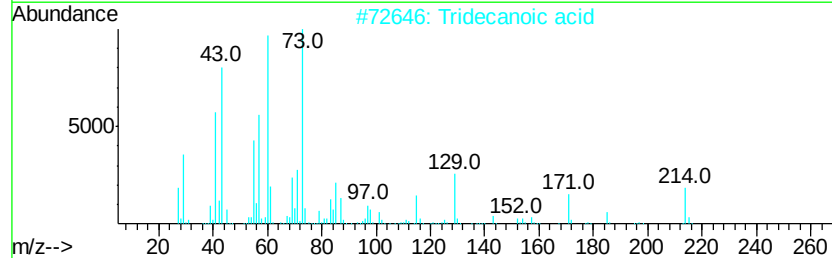
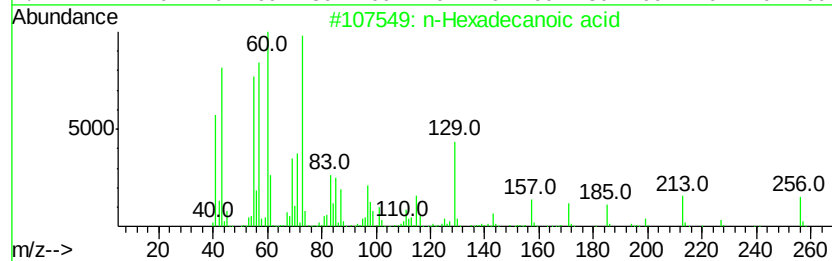
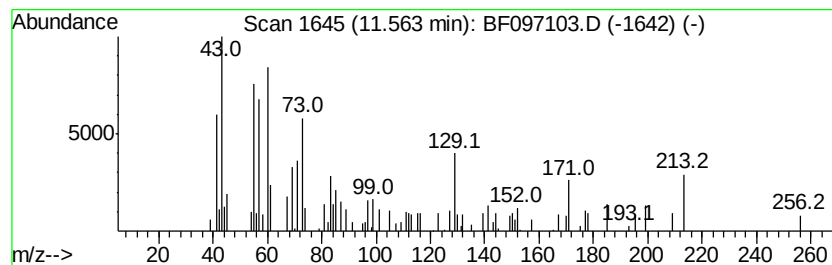
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	2.55 ng	67281	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2	Tridecanoic acid	214	C13H26O2	000638-53-9	72
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
Data File : BF097103.D
Acq On : 27 Jul 2017 4:10
Operator : SJ/JU
Sample : I4415-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-02-072417

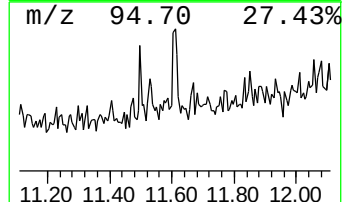
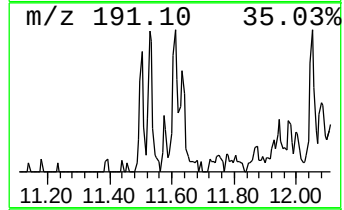
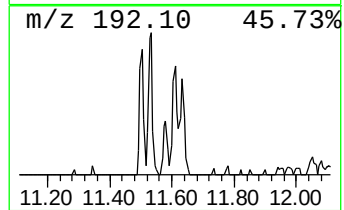
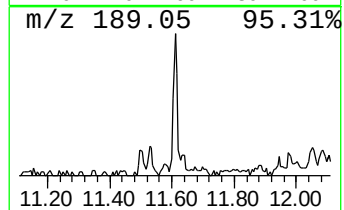
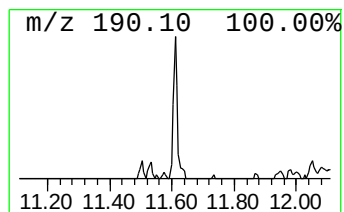
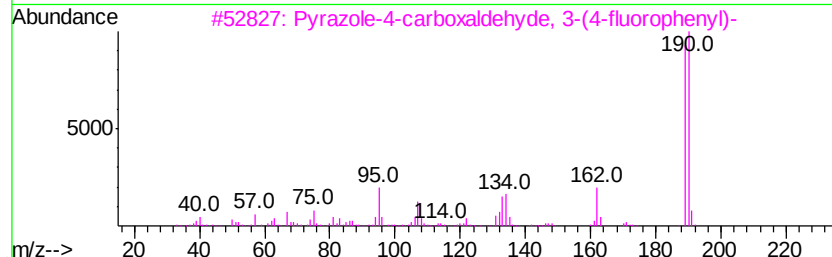
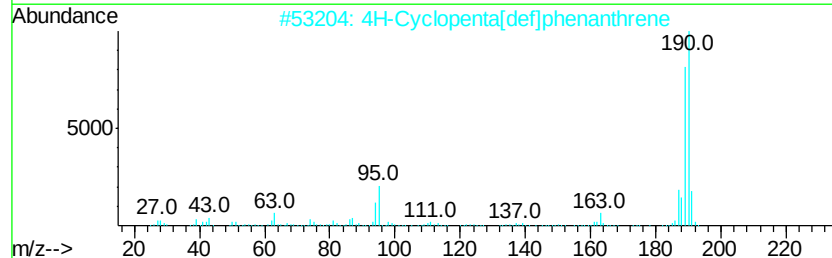
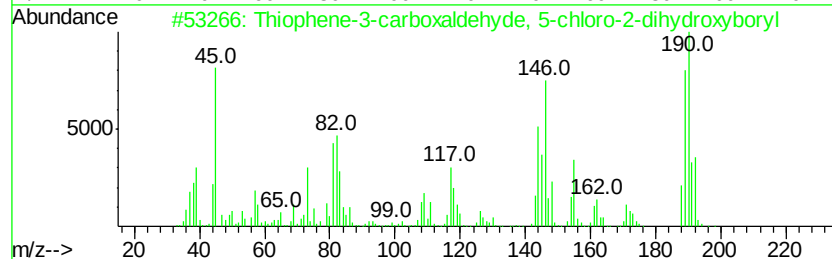
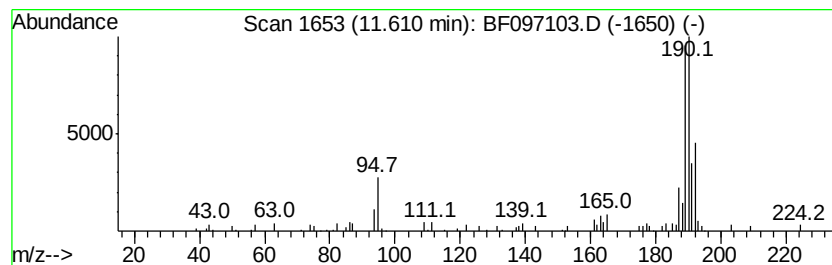
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Thiophene-3-carboxaldehyde,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.61	2.02 ng	53422	Phenanthrene-d10	11.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	72
2		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
3		Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	50
4		Carbonic acid, 2-formyl-4,6-dich...	276	C11H10Cl2O4	1000331-39-3	37
5		Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	36



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097103.D
Acq On : 27 Jul 2017 4:10
Operator : SJ/JU
Sample : I4415-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

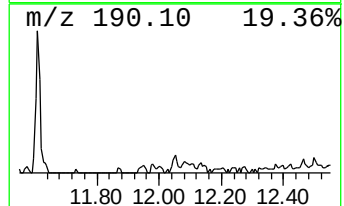
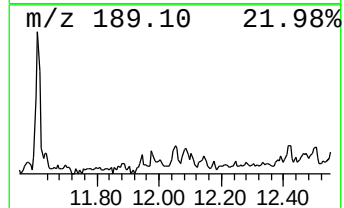
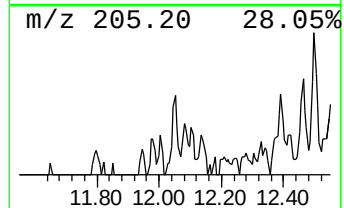
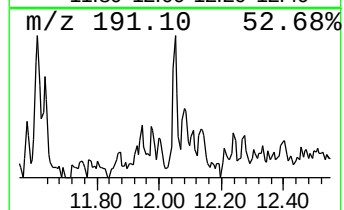
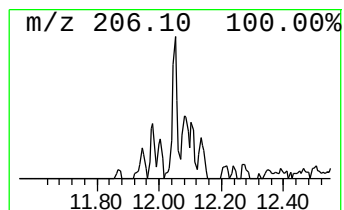
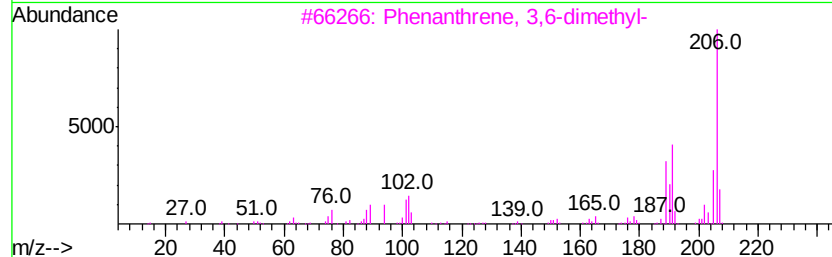
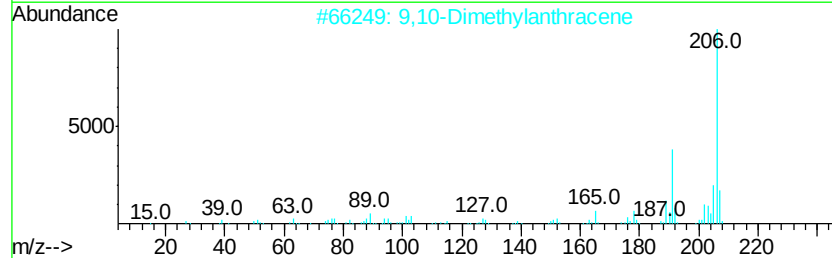
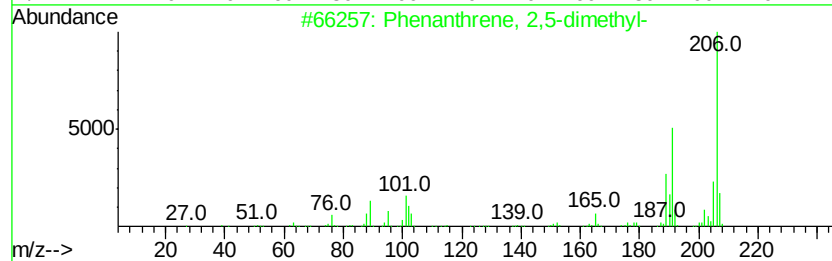
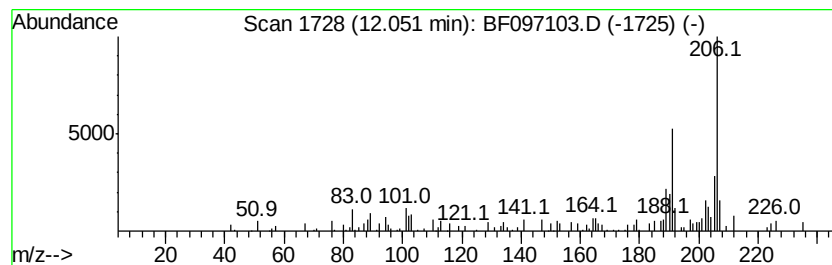
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenanthrene, 2,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.05	2.69 ng	71215	Phenanthrene-d10		11.00
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	90
2	9,10-Dimethylantracene	206	C16H14	000781-43-1	87
3	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	81
4	di-p-Tolylacetylene	206	C16H14	002789-88-0	81
5	1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
Data File : BF097103.D
Acq On : 27 Jul 2017 4:10
Operator : SJ/JU
Sample : I4415-01
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ALS Vial : 24 Sample Multiplier: 1

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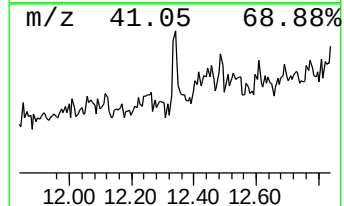
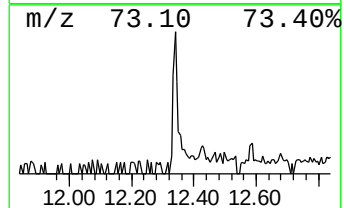
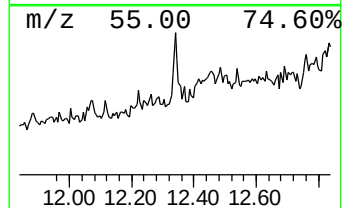
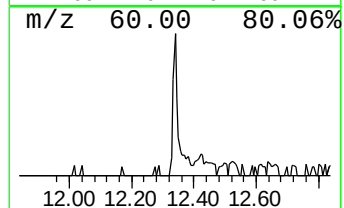
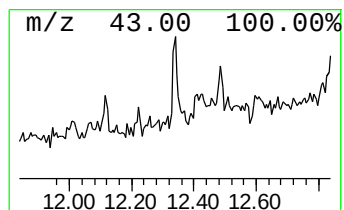
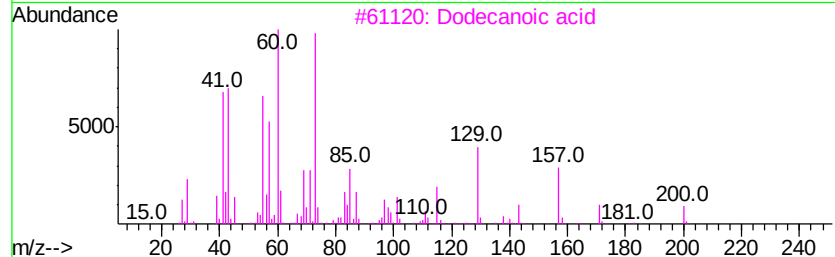
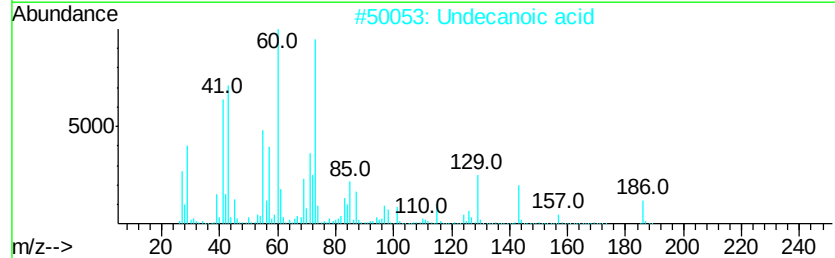
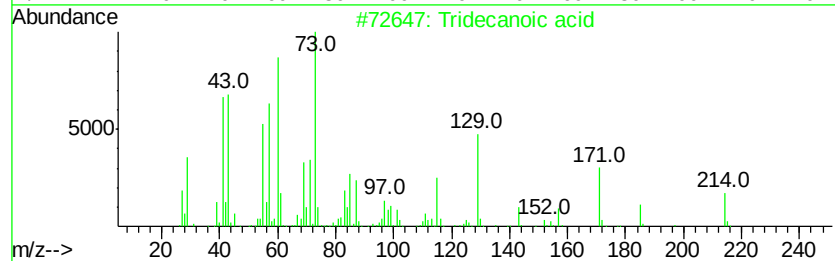
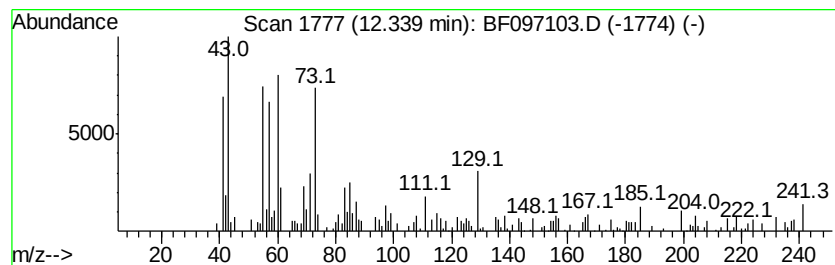
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	4.18 ng	115827	Chrysene-d12	13.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	68
2		Undecanoic acid	186	C11H22O2	000112-37-8	59
3		Dodecanoic acid	200	C12H24O2	000143-07-7	59
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5		n-Decanoic acid	172	C10H20O2	000334-48-5	52



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
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Acq On : 27 Jul 2017 4:10
Operator : SJ/JU
Sample : I4415-01
Misc :
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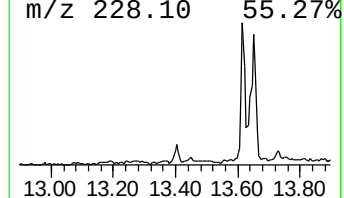
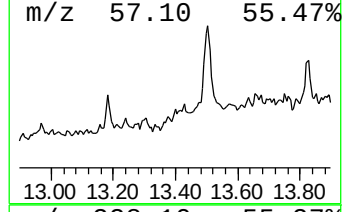
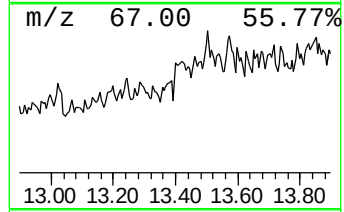
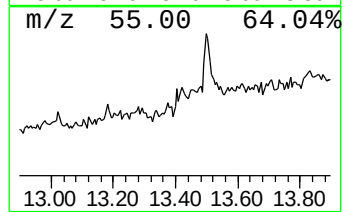
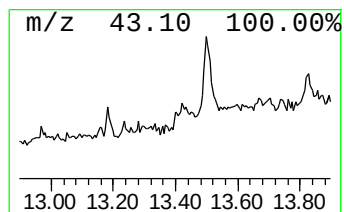
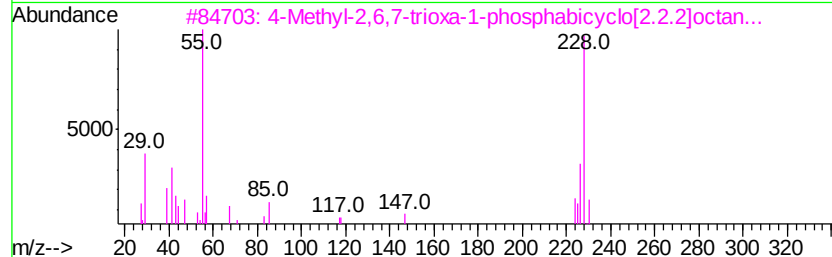
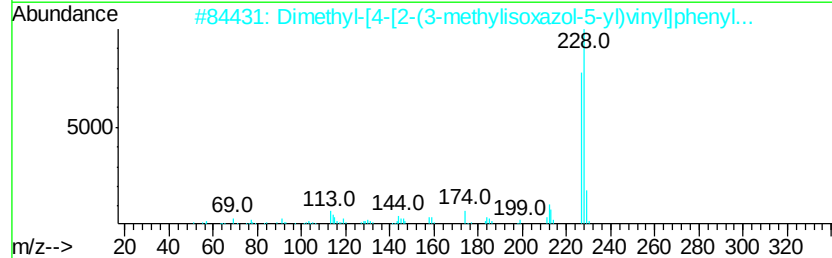
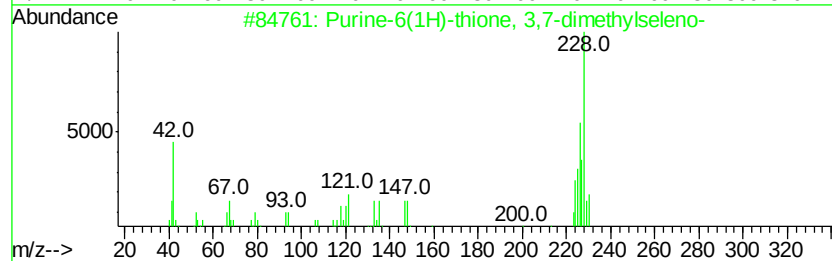
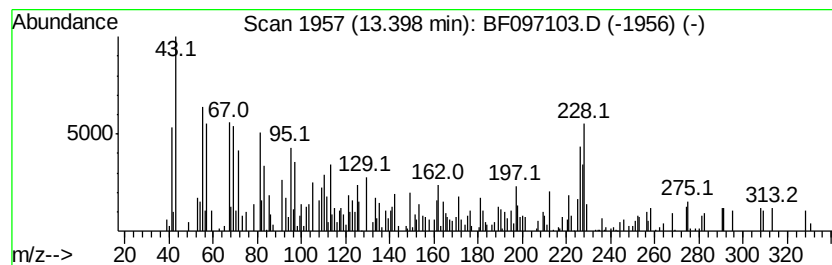
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown13.40 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.40	2.12 ng	58819	Chrysene-d12	13.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Purine-6(1H)-thione, 3,7-dimethy...	228	C7H8N4Se	023663-58-3	25
2	Dimethyl-[4-[2-(3-methylisoxazol...	228	C14H16N2O	1000306-39-6	25
3	4-Methyl-2,6,7-trioxa-1-phosphab...	228	C5H9O3PSe	067471-54-9	14
4	6-Phenylthio-1,2,4-triazolo(4,3-...	228	C11H8N4S	099974-48-8	12
5	1-Ethyl-3-(pyrrolidin-2-ylidene)...	228	C14H16N2O	1000260-86-3	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
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Acq On : 27 Jul 2017 4:10
Operator : SJ/JU
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Misc :
ALS Vial : 24 Sample Multiplier: 1

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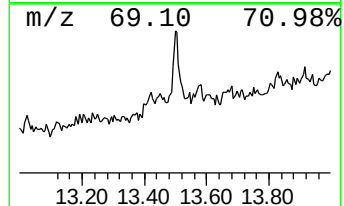
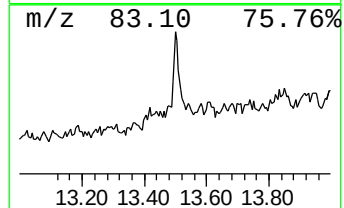
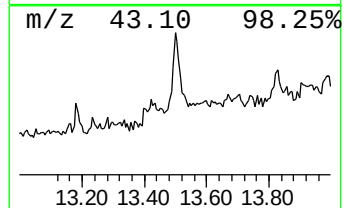
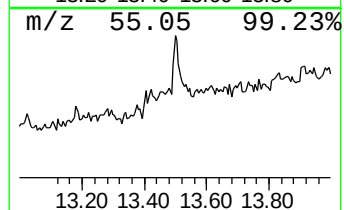
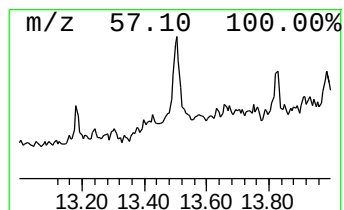
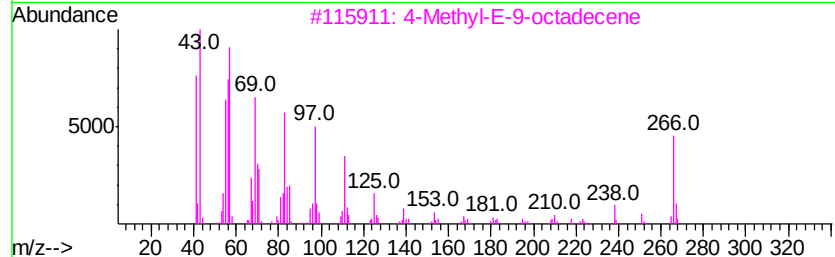
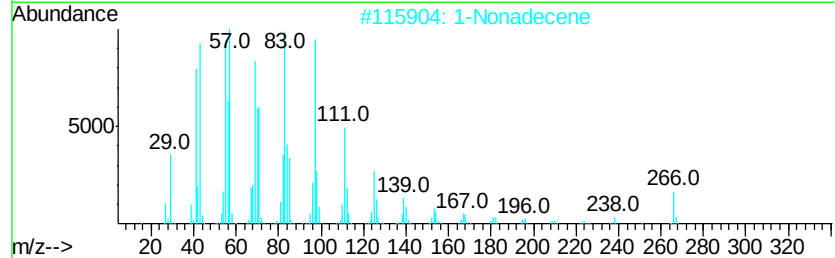
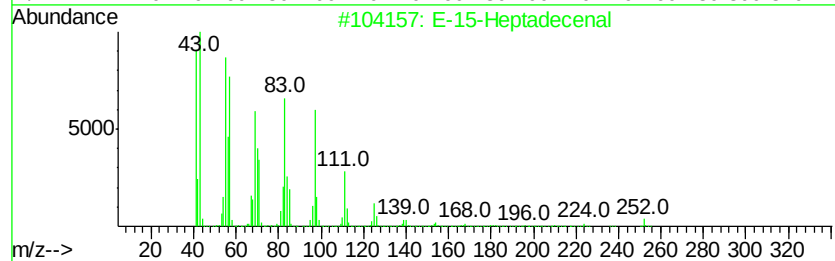
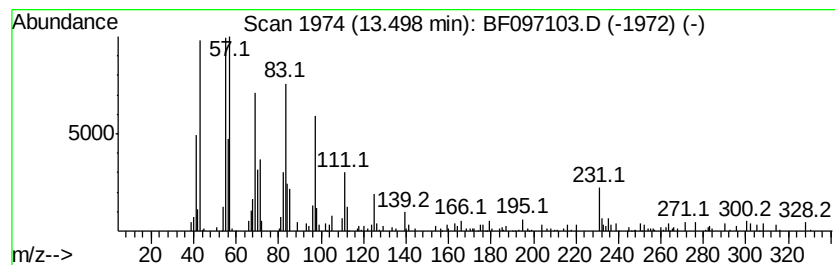
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 E-15-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	5.61 ng	155421	Chrysene-d12	13.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			E-15-Heptadecenal	252	C17H32O	1000130-97-9	90
2			1-Nonadecene	266	C19H38	018435-45-5	90
3			4-Methyl-E-9-octadecene	266	C19H38	1000130-87-1	90
4			1-Octadecene	252	C18H36	000112-88-9	86
5			Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	68



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072617\
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Misc :
ALS Vial : 24 Sample Multiplier: 1

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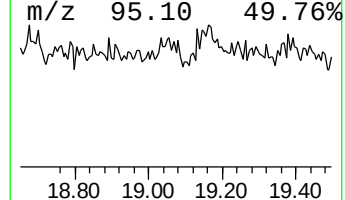
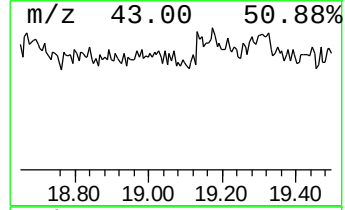
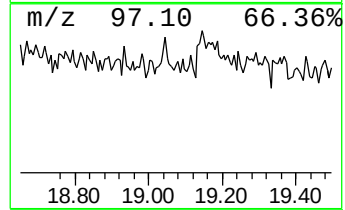
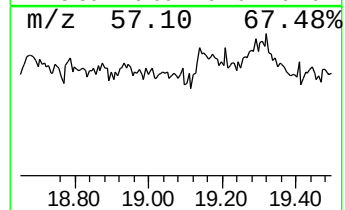
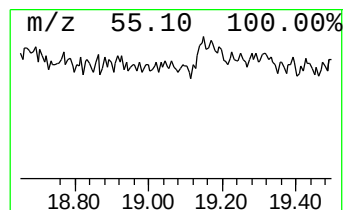
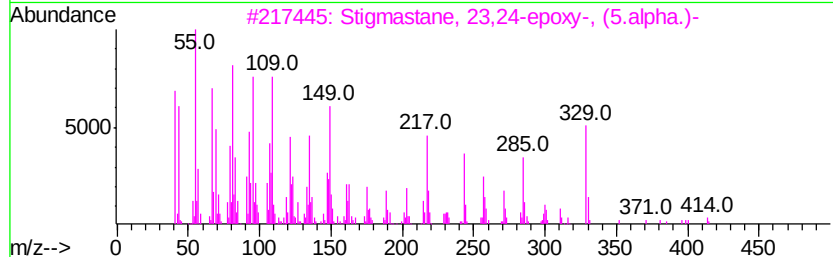
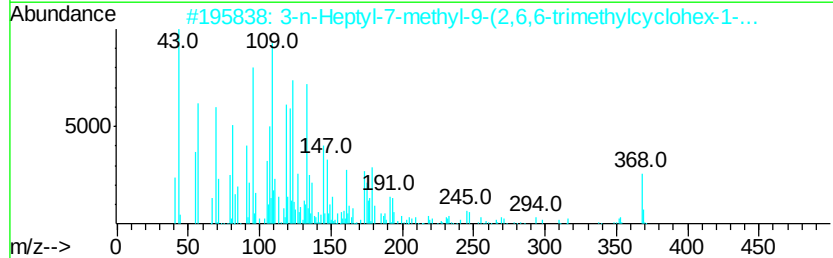
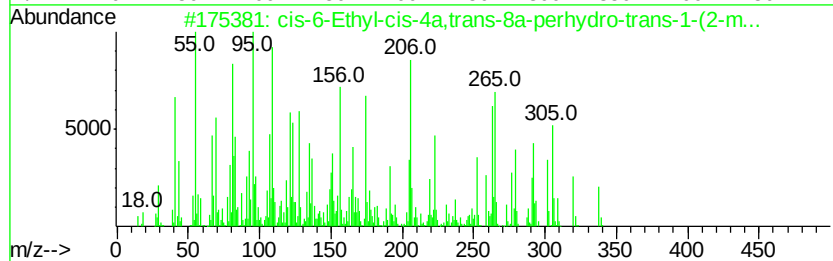
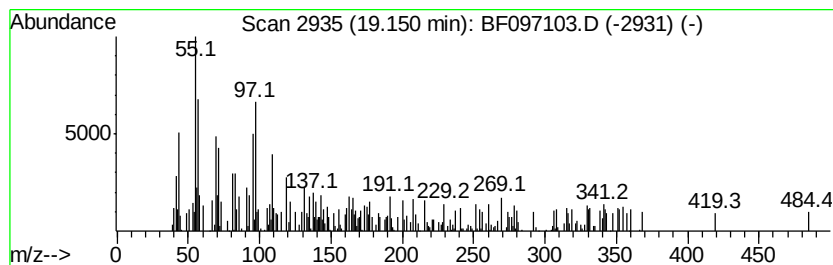
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown19.15 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.15	9.25 ng	90609	Perylene-d12	14.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-6-Ethyl-cis-4a,trans-8a-perh...	338	C20H34O4	106864-11-3	27
2		3-n-Heptyl-7-methyl-9-(2,6,6-tri...	368	C26H40O	1000216-09-3	15
3		Stigmastane, 23,24-epoxy-, (5.alpha...	414	C29H50O	054411-91-5	10
4		Tetraacetyl-.alpha.-D-glucofuros...	488	C20H24O12S	1000125-84-5	10
5		Fumaric acid, 1-cyclopentylethyl...	464	C29H52O4	1000345-18-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072617\
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 Acq On : 27 Jul 2017 4:10
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Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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
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2-Pentanone, 4-hy...	4.63	8.3 ng		234879	1	6.50	562374	20.0
unknown6.27	6.27	73.6 ng		2068360	1	6.50	562374	20.0
Hexacosane	10.45	2.2 ng		58091	4	11.00	528526	20.0
n-Hexadecanoic acid	11.56	2.5 ng		67281	4	11.00	528526	20.0
Thiophene-3-carbo...	11.61	2.0 ng		53422	4	11.00	528526	20.0
Phenanthrene, 2,5...	12.05	2.7 ng		71215	4	11.00	528526	20.0
Tridecanoic acid	12.34	4.2 ng		115827	5	13.63	554466	20.0
unknown13.40	13.40	2.1 ng		58819	5	13.63	554466	20.0
E-15-Heptadecenal	13.50	5.6 ng		155421	5	13.63	554466	20.0
unknown19.15	19.15	9.3 ng		90609	6	14.99	195972	20.0