

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052916\
 Data File : BF087578.D
 Acq On : 31 May 2016 7:20
 Operator : UM/SJ
 Sample : H3323-02
 Misc :
 ALS Vial : 96 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02-COMP

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-BF052316.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	4.707	271	273	297	rBV	96036	360495	10.89%	1.180%
2	5.381	329	332	362	rBV	1112607	3047519	92.04%	9.974%
3	7.039	475	477	483	rBV	1889108	2836375	85.66%	9.283%
4	7.130	483	485	495	rVB	1900064	3311231	100.00%	10.838%
5	7.473	512	515	526	rBV	451477	803666	24.27%	2.630%
6	7.702	532	535	550	rVB	1650062	2299649	69.45%	7.527%
7	8.387	593	595	616	rBV	1191903	1932612	58.37%	6.325%
8	9.496	690	692	707	rBV	473289	1006737	30.40%	3.295%
9	11.279	845	848	858	rBV	2252444	3050460	92.12%	9.984%
10	11.485	863	866	870	rVB	24787	39751	1.20%	0.130%
11	11.976	907	909	917	rVB	145307	264819	8.00%	0.867%
12	12.331	937	940	944	rBV	575729	930191	28.09%	3.044%
13	12.719	968	974	976	rBV4	13028	33781	1.02%	0.111%
14	13.154	1009	1012	1015	rVB	51013	63662	1.92%	0.208%
15	13.519	1041	1044	1048	rBV2	20672	48053	1.45%	0.157%
16	13.622	1051	1053	1067	rVV2	747393	1476337	44.59%	4.832%
17	13.931	1078	1080	1084	rBV	56463	108698	3.28%	0.356%
18	14.662	1140	1144	1146	rBV2	42120	63613	1.92%	0.208%
19	14.742	1149	1151	1153	rBV	495327	749759	22.64%	2.454%
20	14.788	1153	1155	1161	rVB	134076	255744	7.72%	0.837%
21	14.891	1162	1164	1168	rVV	25848	42732	1.29%	0.140%
22	15.337	1201	1203	1207	rVB	30750	37366	1.13%	0.122%
23	15.554	1219	1222	1224	rBV	35317	48777	1.47%	0.160%
24	15.600	1224	1226	1231	rVB	33082	48887	1.48%	0.160%
25	15.702	1231	1235	1243	rBV3	52125	185299	5.60%	0.606%
26	15.942	1254	1256	1259	rBV	28178	40522	1.22%	0.133%
27	16.000	1259	1261	1266	rVB2	26062	52876	1.60%	0.173%
28	16.354	1289	1292	1294	rBV2	27139	57347	1.73%	0.188%
29	16.491	1300	1304	1305	rBV2	18847	33916	1.02%	0.111%
30	16.560	1308	1310	1315	rBV	241944	422794	12.77%	1.384%
31	16.857	1334	1336	1340	rBV	279071	441289	13.33%	1.444%
32	16.925	1340	1342	1344	rVB	238563	247376	7.47%	0.810%
33	16.994	1344	1348	1350	rBV2	36873	77804	2.35%	0.255%
34	17.040	1350	1352	1354	rBV2	32131	47488	1.43%	0.155%

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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-BF052316.M
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35	17.085	1354	1356	1359	rBV	2033365	2273882	68.67%	7.442%
36	17.291	1370	1374	1377	rBV6	28365	93638	2.83%	0.306%
37	17.337	1377	1378	1382	rVB	39793	55947	1.69%	0.183%
38	17.474	1387	1390	1393	rBV2	67823	126922	3.83%	0.415%
39	17.588	1398	1400	1402	rVV	28776	39456	1.19%	0.129%
40	17.634	1402	1404	1406	rVB2	32361	46408	1.40%	0.152%
41	17.748	1411	1414	1416	rBV	239453	257073	7.76%	0.841%
42	17.851	1421	1423	1426	rBV2	126897	164532	4.97%	0.539%
43	17.908	1426	1428	1430	rVV	52159	66497	2.01%	0.218%
44	18.331	1464	1465	1473	rBV3	61358	145851	4.40%	0.477%
45	18.457	1473	1476	1485	rBV2	530849	1253287	37.85%	4.102%
46	18.731	1498	1500	1504	rBV2	67877	108985	3.29%	0.357%
47	19.120	1532	1534	1537	rVB2	66429	73686	2.23%	0.241%
48	19.463	1562	1564	1565	rBV	106773	143209	4.32%	0.469%
49	19.749	1587	1589	1595	rBV	123373	230887	6.97%	0.756%
50	19.840	1595	1597	1599	rBV	110610	147197	4.45%	0.482%
51	20.103	1619	1620	1622	rBV	97247	149369	4.51%	0.489%
52	20.149	1622	1624	1626	rBV	263760	385928	11.66%	1.263%
53	20.629	1664	1666	1673	rVB4	159107	322850	9.75%	1.057%

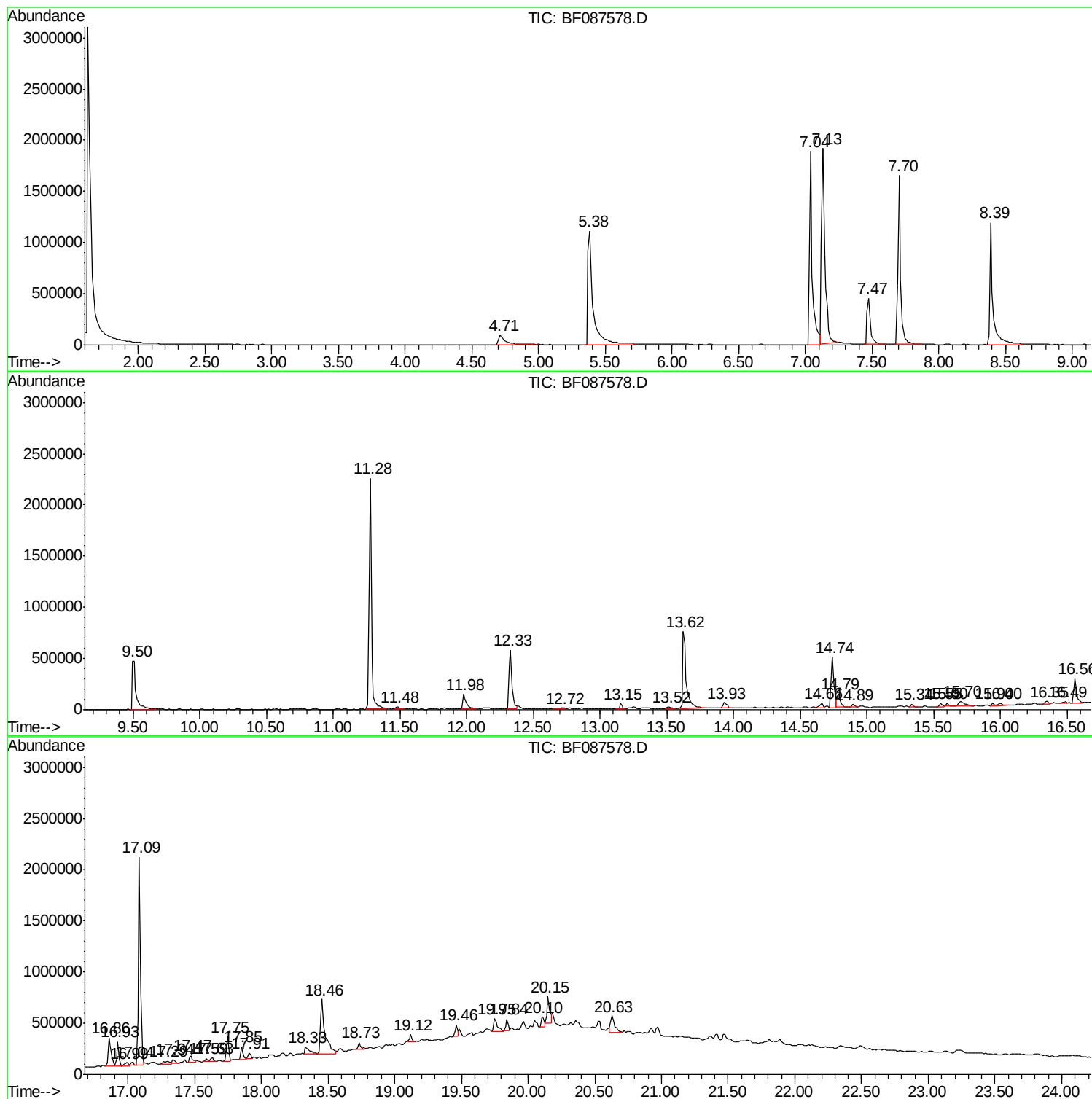
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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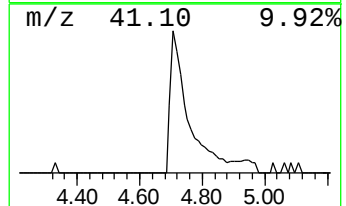
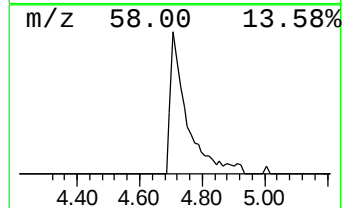
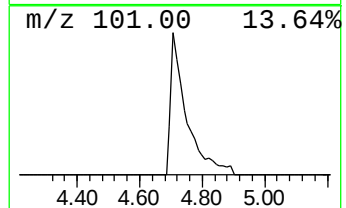
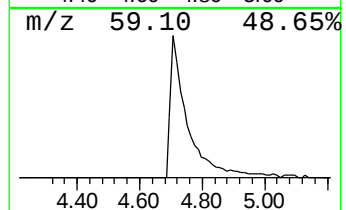
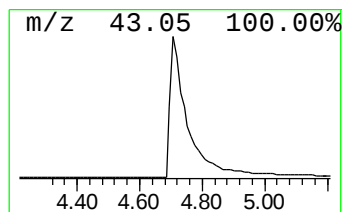
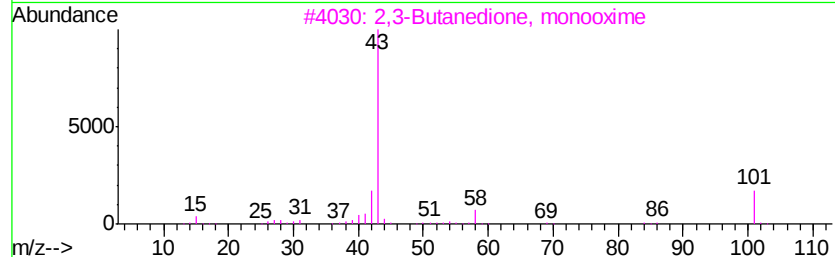
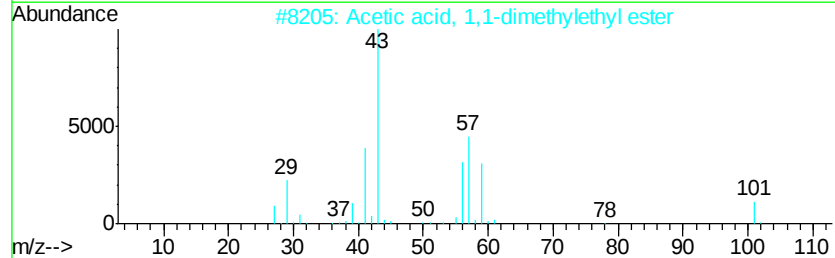
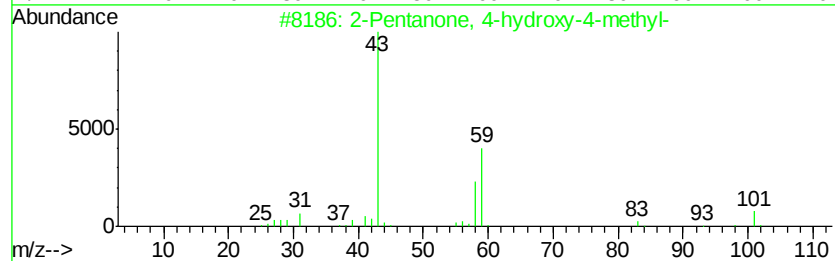
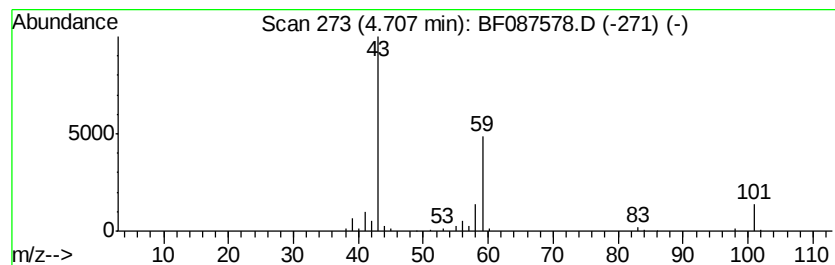
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	8.97 ng	360495	1,4-Dichlorobenzene-d4	7.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5			Diacetamide	101	C4H7NO2	000625-77-4	9



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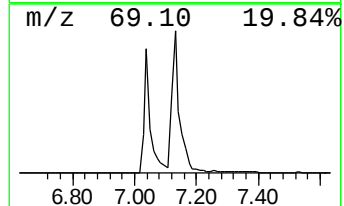
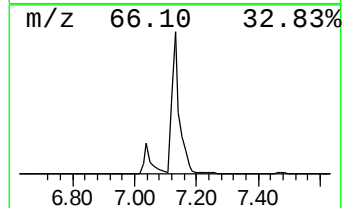
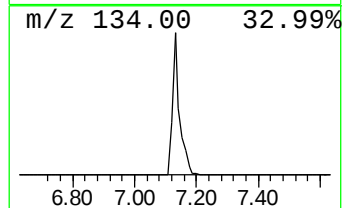
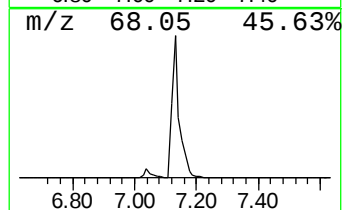
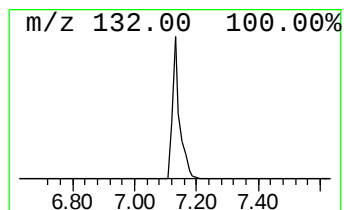
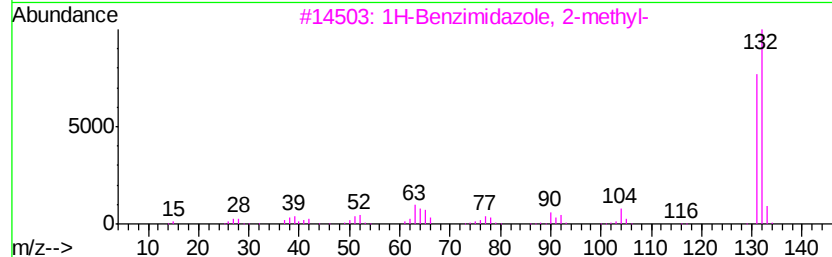
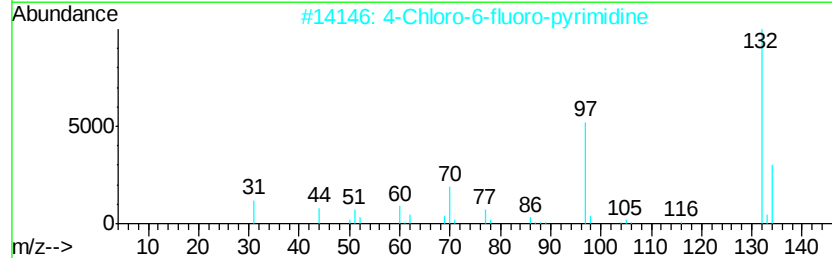
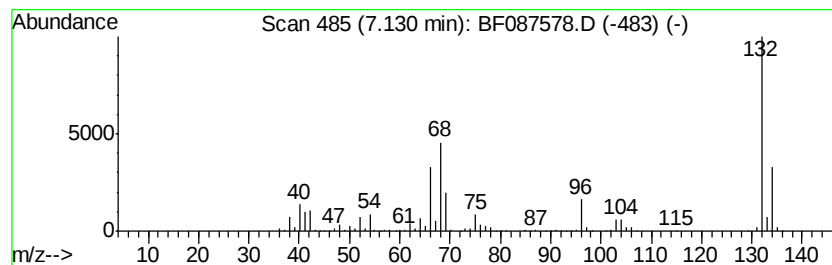
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.13	82.40 ng	3311230	1,4-Dichlorobenzene-d4	7.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



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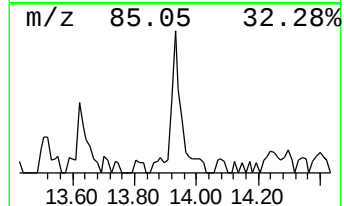
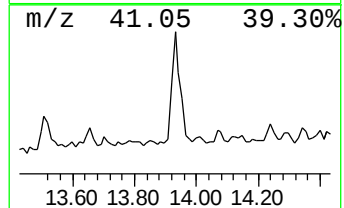
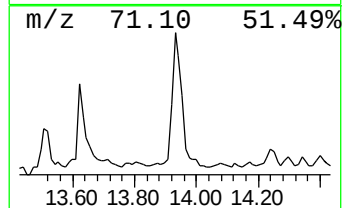
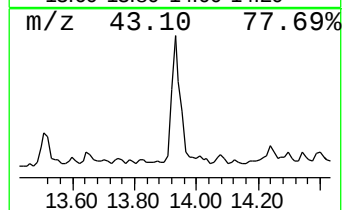
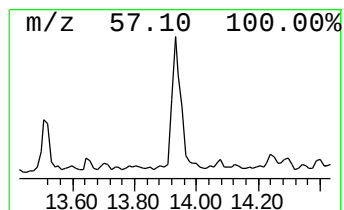
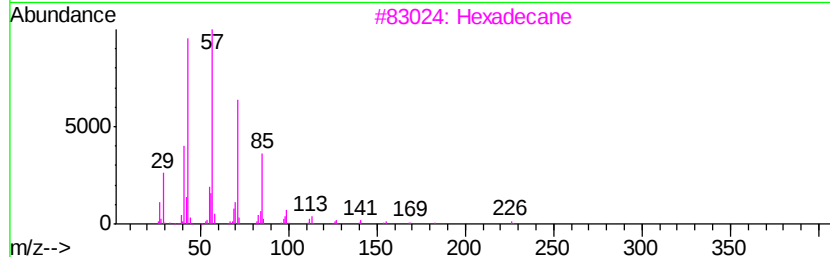
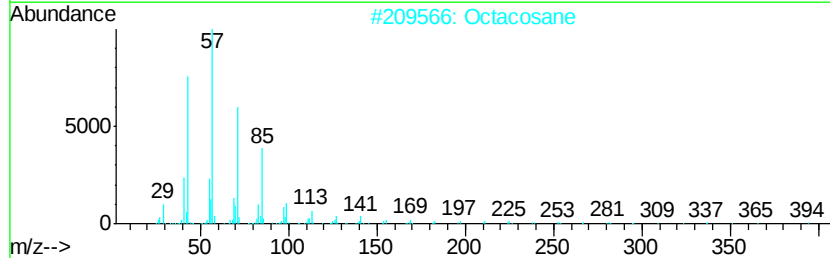
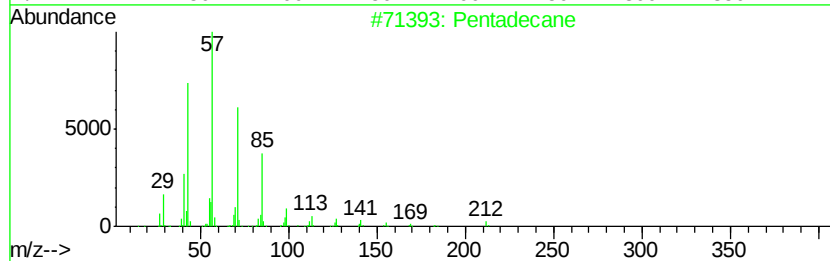
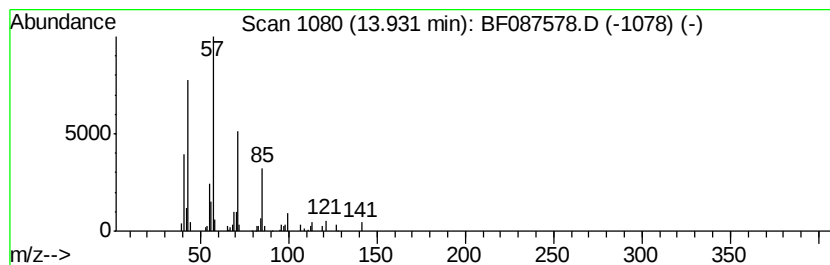
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	2.90 ng	108698	Phenanthrene-d10	14.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	86
2	Octacosane		394	C28H58	000630-02-4	86
3	Hexadecane		226	C16H34	000544-76-3	86
4	Tridecane		184	C13H28	000629-50-5	80
5	Eicosane		282	C20H42	000112-95-8	80



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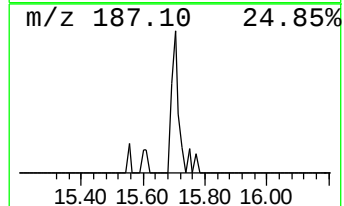
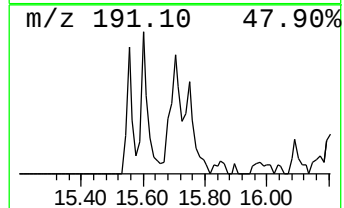
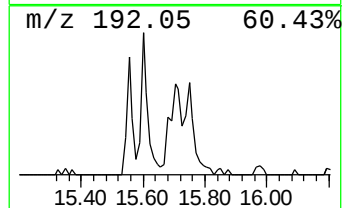
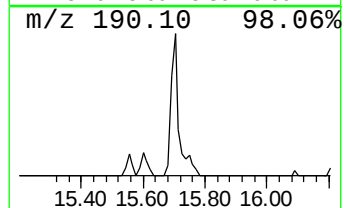
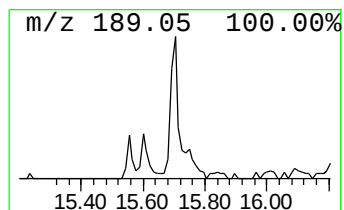
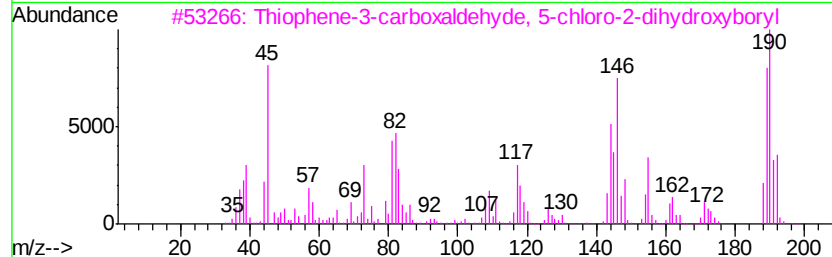
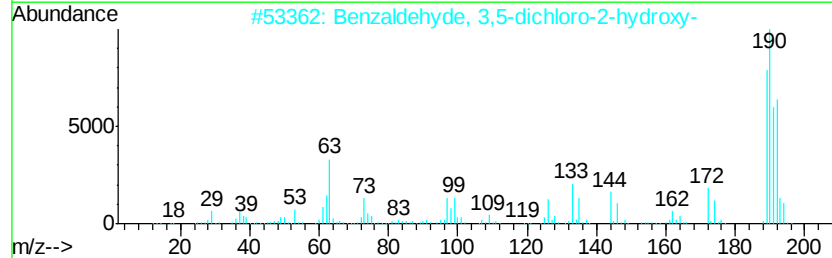
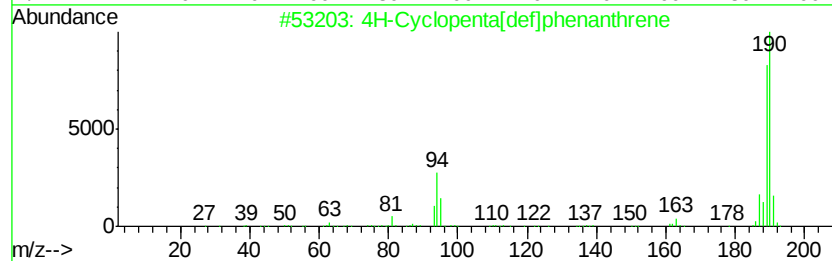
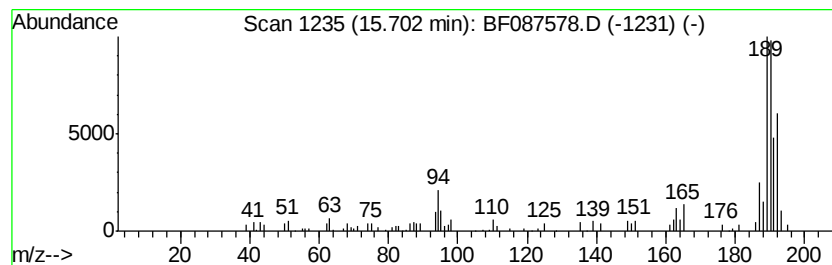
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.70	4.94 ng	185299	Phenanthrene-d10	14.74	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	50
3	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
4	6H-Cyclobuta[flk]phenanthrene	190	C15H10	083469-43-6	49
5	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	43



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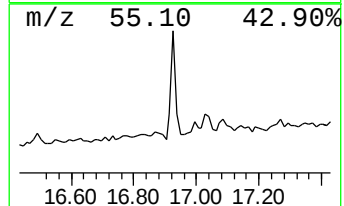
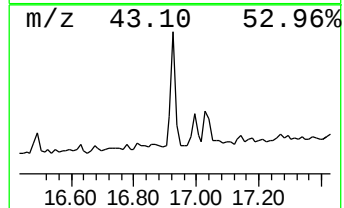
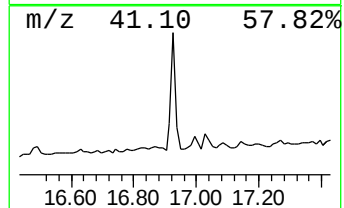
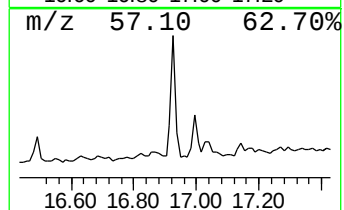
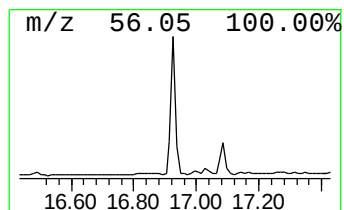
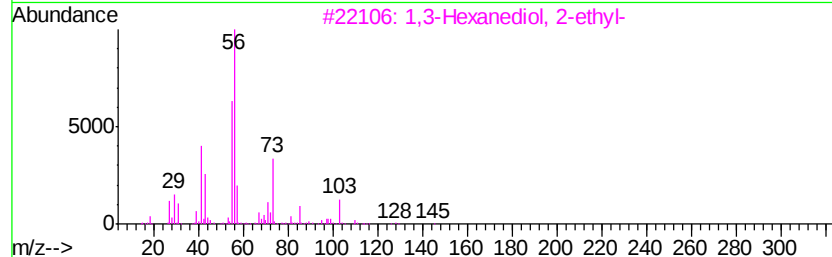
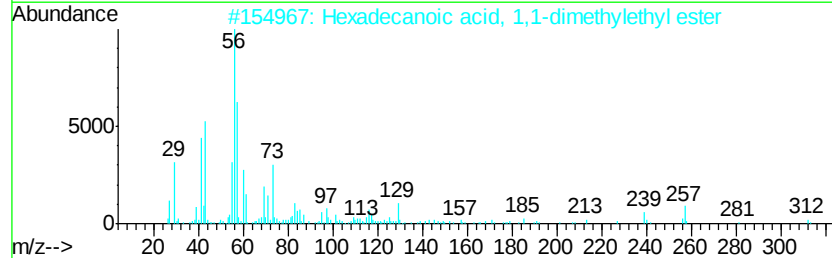
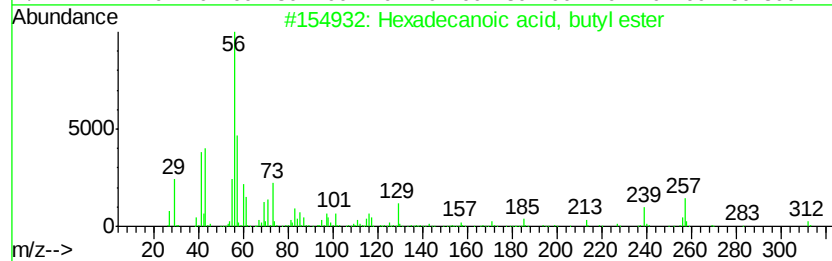
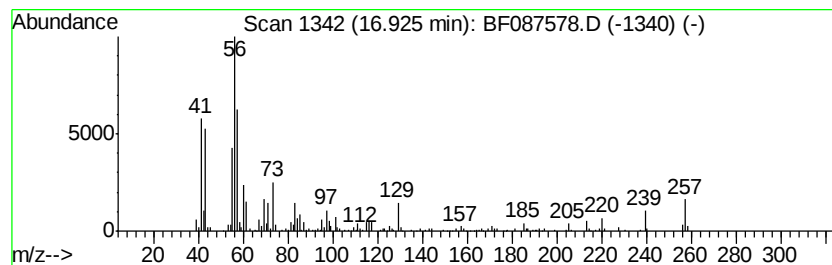
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	3.95 ng	247376	Chrysene-d12	18.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
3		1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	43
4		1-Pentadecene, 2-methyl-	224	C16H32	029833-69-0	38
5		2-Undecene, 10-methyl-	168	C12H24	1000061-83-3	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
Data File : BF087578.D
Acq On : 31 May 2016 7:20
Operator : UM/SJ
Sample : H3323-02
Misc :
ALS Vial : 96 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-COMP

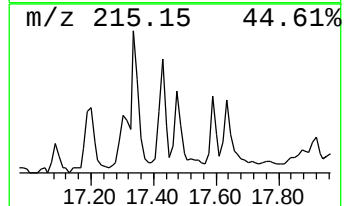
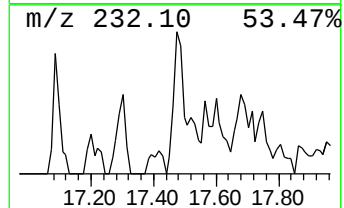
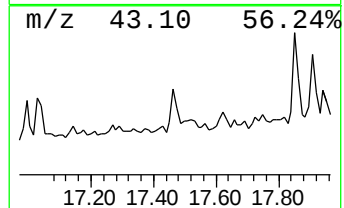
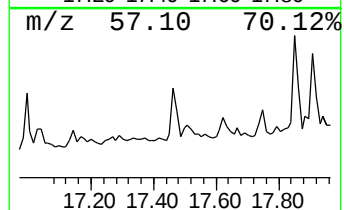
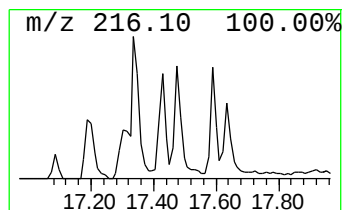
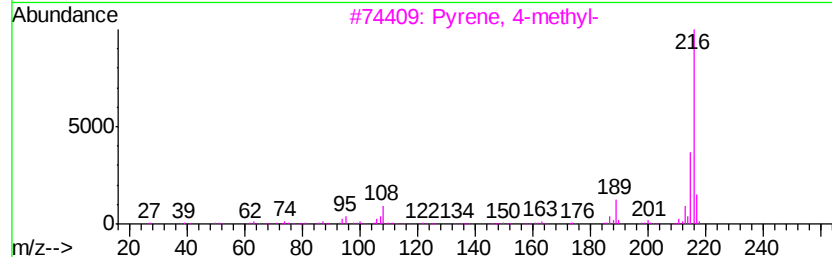
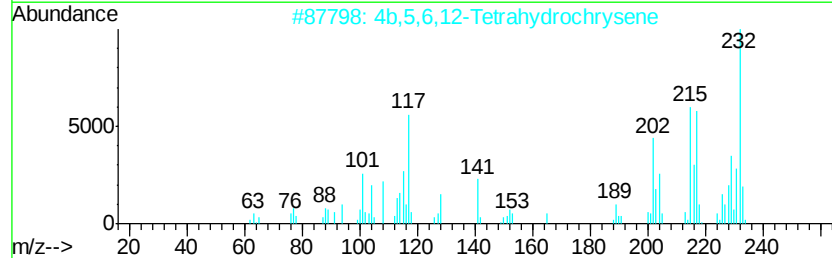
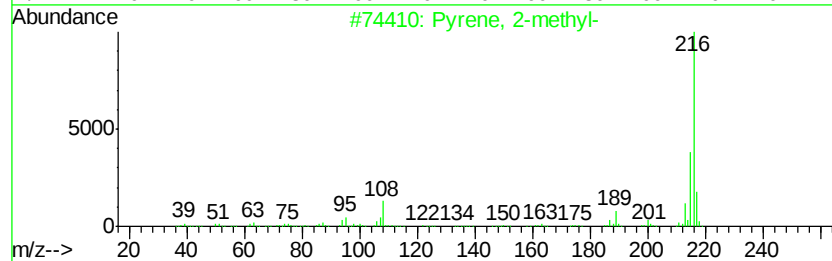
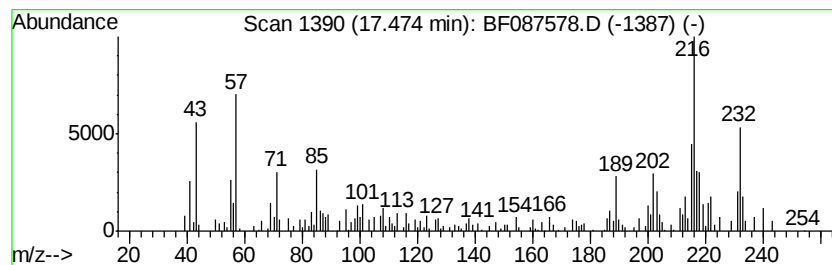
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pyrene, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.47	2.03 ng	126922	Chrysene-d12	18.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	64
2		4b,5,6,12-Tetrahydrochrysene	232	C18H16	031570-60-2	55
3		Pyrene, 4-methyl-	216	C17H12	003353-12-6	50
4		Pyrene, 1-methyl-	216	C17H12	002381-21-7	43
5		5-(2-Propenylidene)-10,11-dihydr...	232	C18H16	024755-73-5	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
Data File : BF087578.D
Acq On : 31 May 2016 7:20
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Misc :
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ClientSampleId :
SB-02-COMP

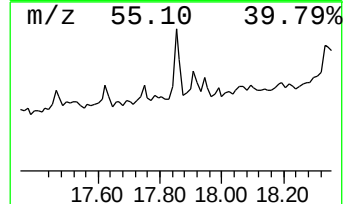
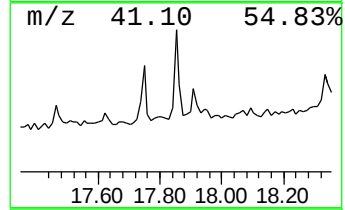
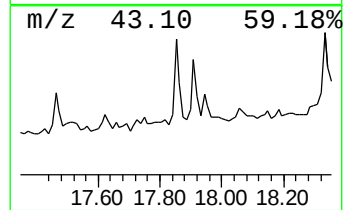
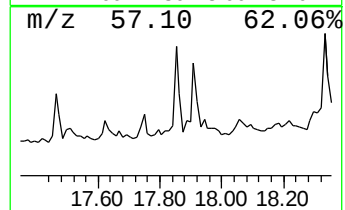
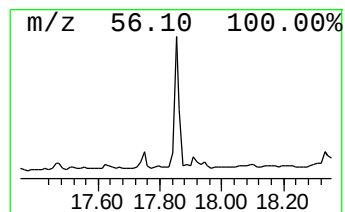
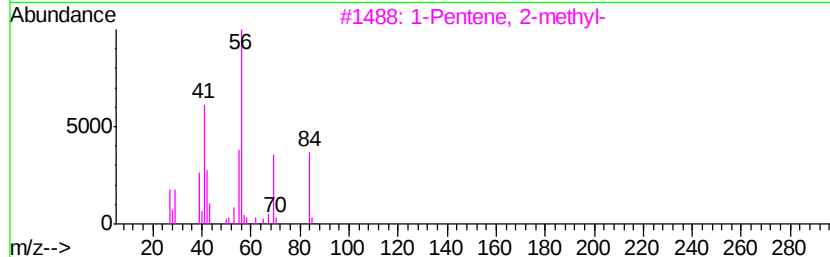
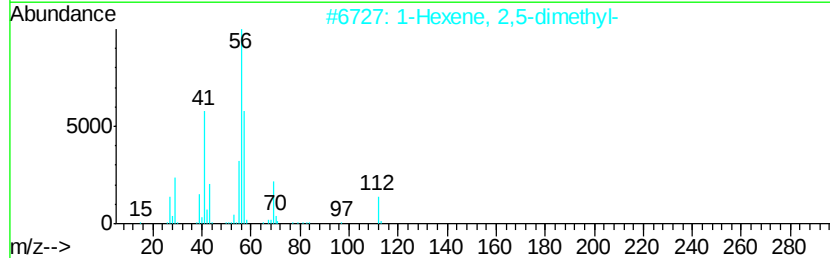
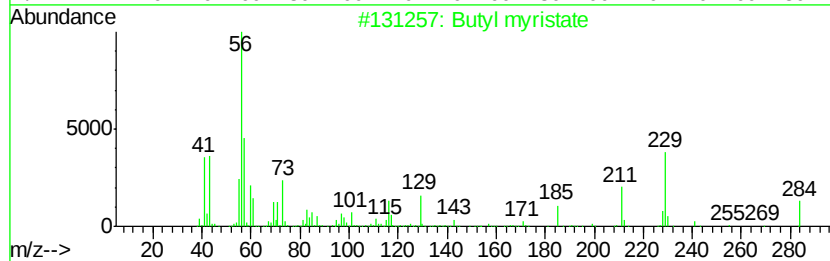
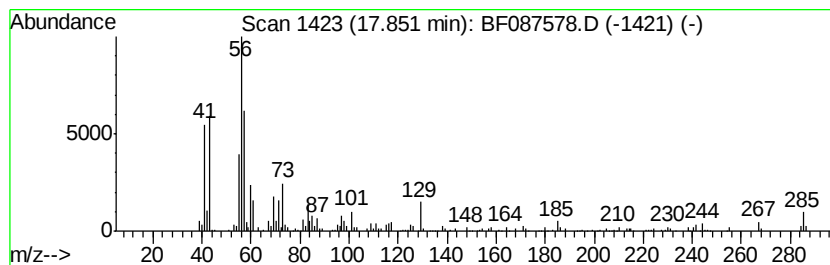
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Butyl myristate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	2.63 ng	164532	Chrysene-d12	18.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butyl myristate	284	C18H36O2	000110-36-1	64
2		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35
3		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	35
4		2-Isopropyl-3-vinylloxirane	112	C7H12O	070777-23-0	35
5		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
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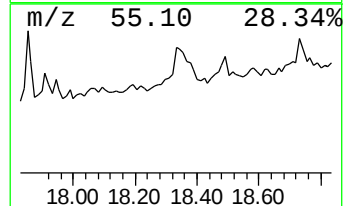
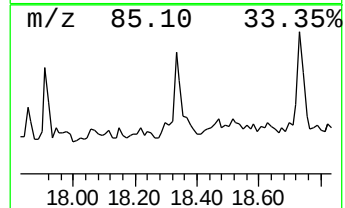
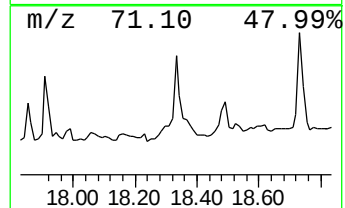
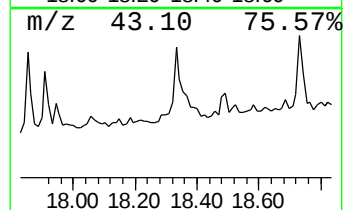
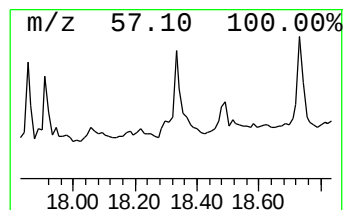
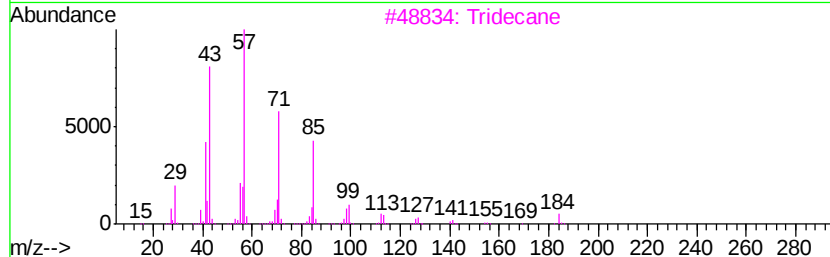
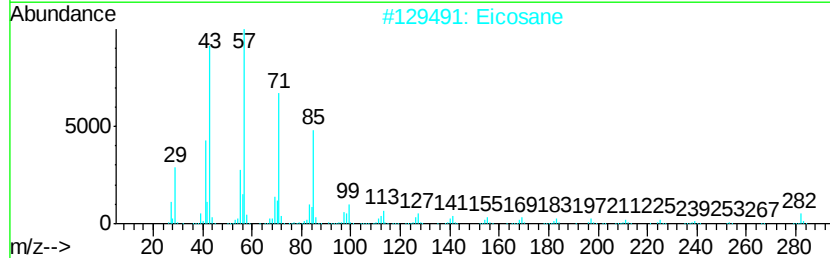
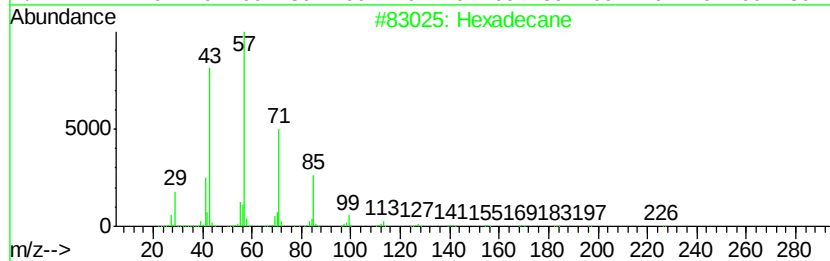
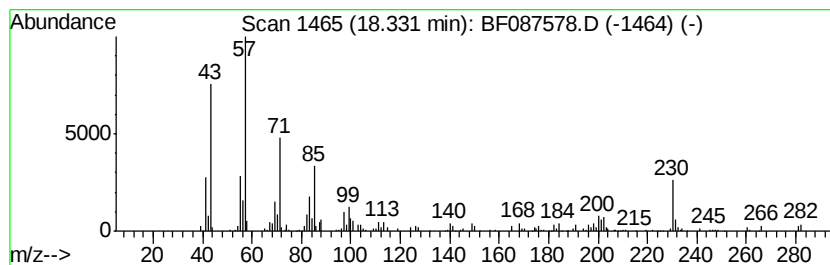
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.33	2.33 ng	145851	Chrysene-d12		18.46
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	83
3	Tridecane	184	C13H28	000629-50-5	78
4	Tetradecane	198	C14H30	000629-59-4	70
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
Data File : BF087578.D
Acq On : 31 May 2016 7:20
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Misc :
ALS Vial : 96 Sample Multiplier: 1

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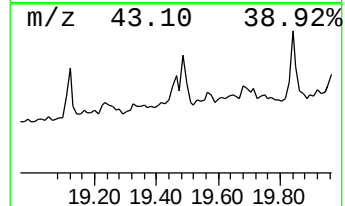
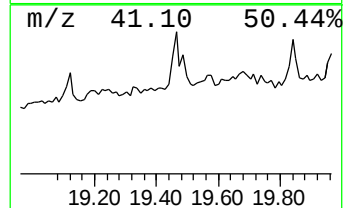
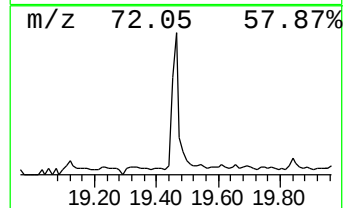
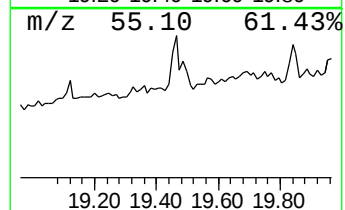
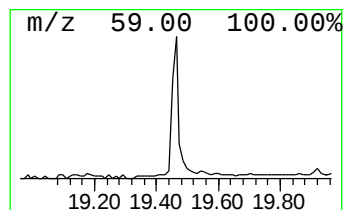
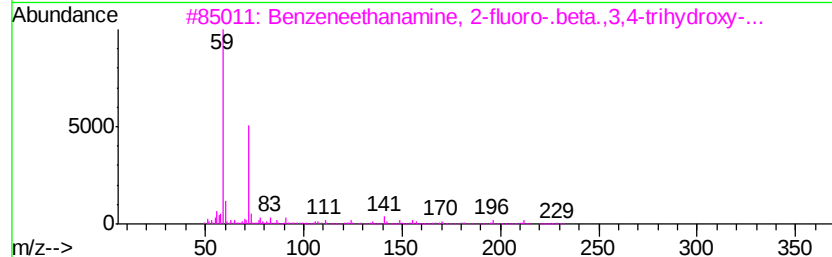
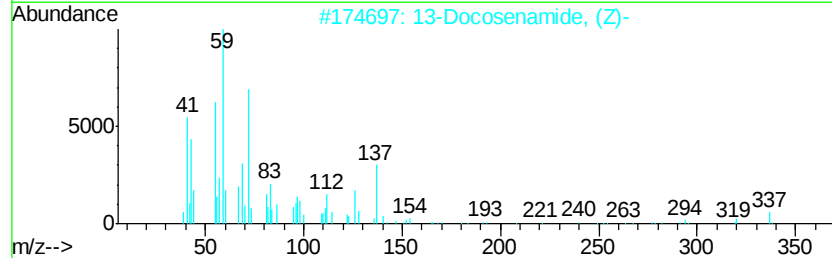
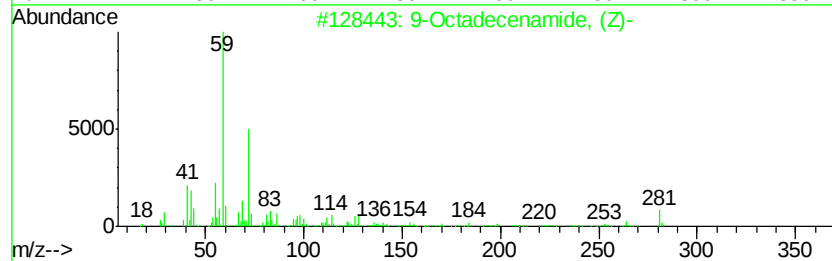
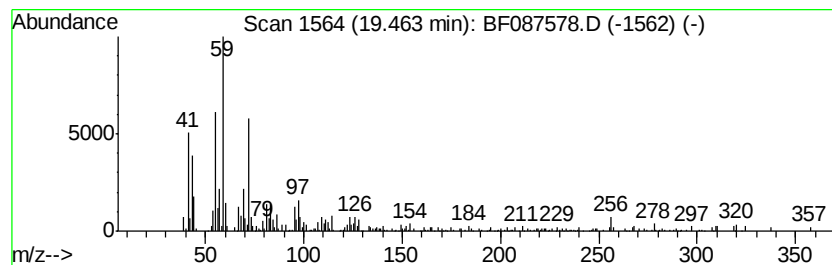
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.46	7.42 ng	143209	Perylene-d12	20.15

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	81
3			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
4			Dodecanamide	199	C12H25NO	001120-16-7	58
5			Octanamide	143	C8H17NO	000629-01-6	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
Data File : BF087578.D
Acq On : 31 May 2016 7:20
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Misc :
ALS Vial : 96 Sample Multiplier: 1

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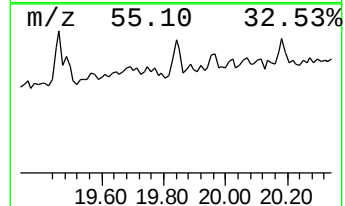
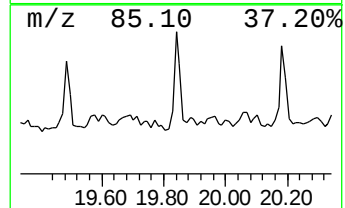
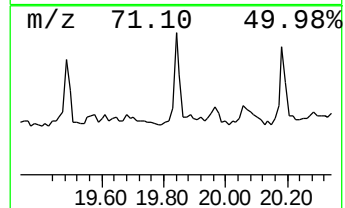
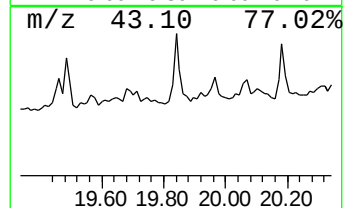
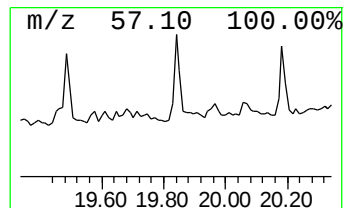
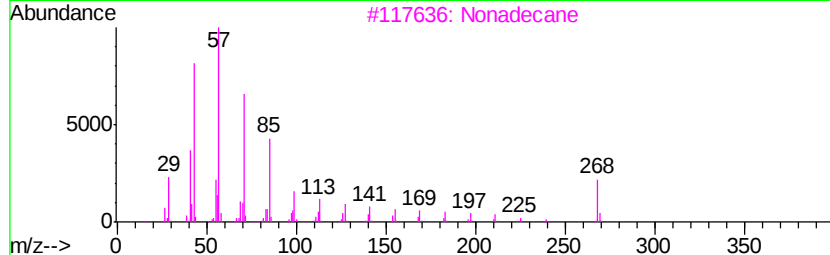
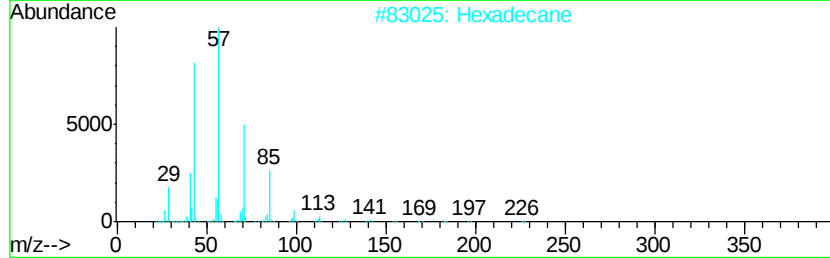
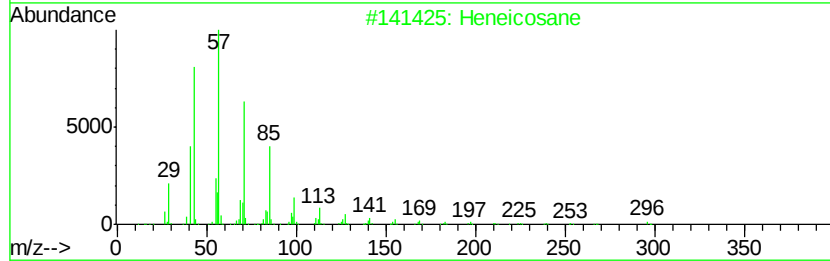
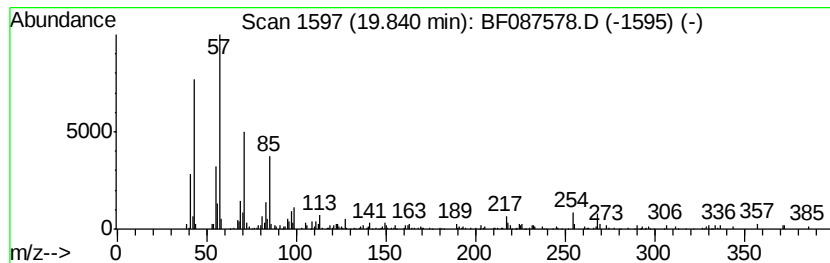
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.84	7.63 ng	147197	Perylene-d12	20.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	95
2		Hexadecane	226	C16H34	000544-76-3	95
3		Nonadecane	268	C19H40	000629-92-5	90
4		Octadecane	254	C18H38	000593-45-3	90
5		Octacosane	394	C28H58	000630-02-4	87



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Acq On : 31 May 2016 7:20
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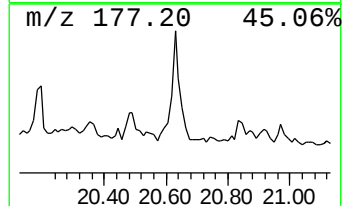
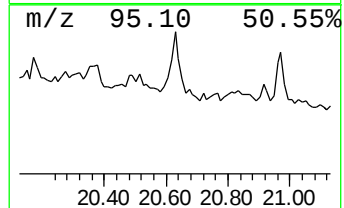
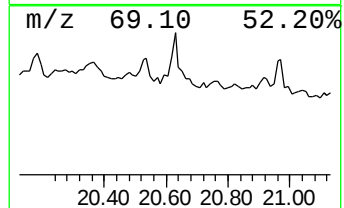
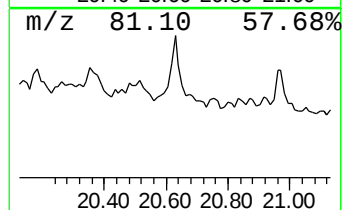
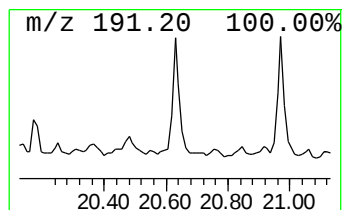
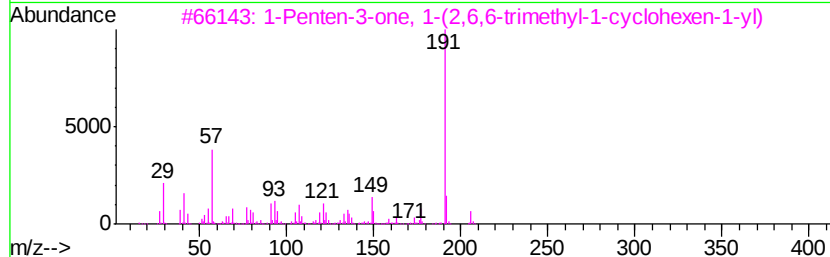
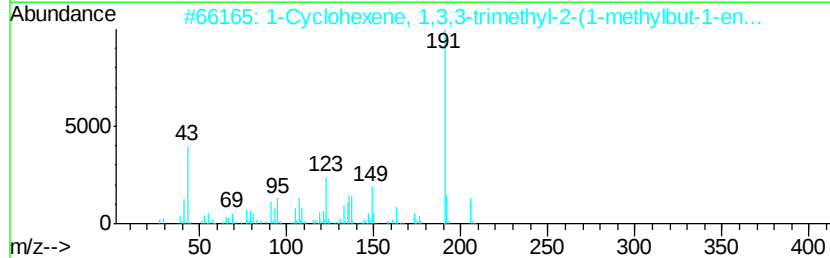
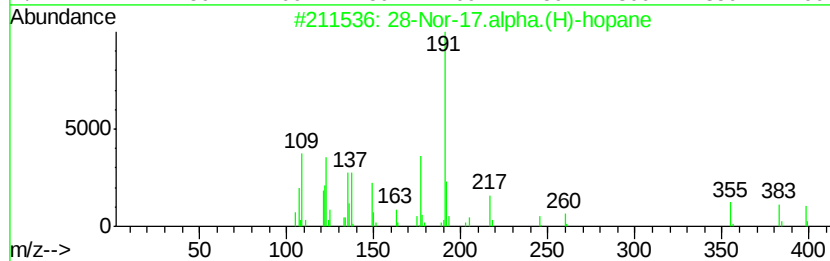
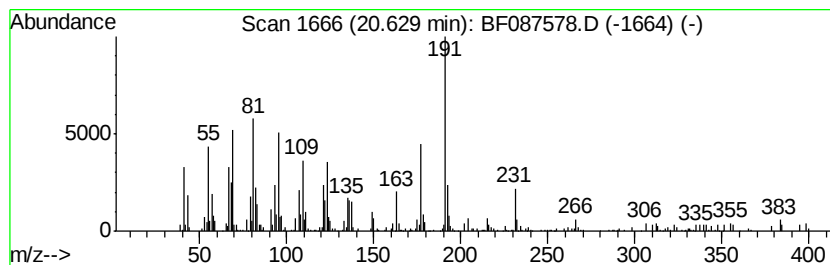
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 28-Nor-17.alpha.(H)-hopane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.63	16.73 ng	322850	Perylene-d12	20.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	90
2		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	43
3		1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38
4		Anthracene, 9-dodecyltetradecahy...	360	C26H48	055401-75-7	37
5		Pyrido[3,4-d]pyridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052916\
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 Acq On : 31 May 2016 7:20
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 Sample : H3323-02
 Misc :
 ALS Vial : 96 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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unknown7.13	7.13	82.4	ng	3311230	1	7.47	803666	20.0
Pentadecane	13.93	2.9	ng	108698	4	14.74	749759	20.0
4H-Cyclopenta[def...	15.70	4.9	ng	185299	4	14.74	749759	20.0
Hexadecanoic acid...	16.93	4.0	ng	247376	5	18.46	1253290	20.0
Pyrene, 2-methyl-	17.47	2.0	ng	126922	5	18.46	1253290	20.0
Butyl myristate	17.85	2.6	ng	164532	5	18.46	1253290	20.0
Hexadecane	18.33	2.3	ng	145851	5	18.46	1253290	20.0
9-Octadecenamide, ...	19.46	7.4	ng	143209	6	20.15	385928	20.0
Heneicosane	19.84	7.6	ng	147197	6	20.15	385928	20.0
28-Nor-17.alpha.(...	20.63	16.7	ng	322850	6	20.15	385928	20.0