

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041918\
 Data File : BF104649.D
 Acq On : 20 Apr 2018 00:42
 Operator : JU/SJ
 Sample : J2455-41
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1-BEDROCK

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-BF040618.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	5.022	494	499	510	rBV	168237	222082	6.30%	0.744%
2	5.428	563	568	571	rBV	3014905	3003816	85.17%	10.065%
3	6.445	736	741	744	rBV	2767070	3082323	87.40%	10.328%
4	6.575	759	763	766	rBV	3055479	3119040	88.44%	10.451%
5	6.804	798	802	805	rBV	970989	762509	21.62%	2.555%
6	6.963	824	829	832	rBV	2761393	2569349	72.85%	8.609%
7	7.369	893	898	901	rBV	1937796	2009590	56.98%	6.733%
8	7.445	907	911	925	rVB3	32762	52981	1.50%	0.178%
9	8.086	1016	1020	1026	rBV	1238148	992971	28.16%	3.327%
10	9.163	1199	1203	1206	rBV	3745695	3526744	100.00%	11.817%
11	9.557	1266	1270	1273	rBV	315649	274755	7.79%	0.921%
12	9.769	1302	1306	1310	rVB	118013	97105	2.75%	0.325%
13	9.839	1315	1318	1327	rVB	1078396	1041918	29.54%	3.491%
14	10.269	1388	1391	1394	rVB	149658	124434	3.53%	0.417%
15	10.486	1422	1428	1430	rBV	50190	60557	1.72%	0.203%
16	10.633	1449	1453	1462	rVB	1934536	1794744	50.89%	6.014%
17	10.739	1468	1471	1479	rBV	173706	175522	4.98%	0.588%
18	11.186	1544	1547	1550	rBV	101284	83116	2.36%	0.278%
19	11.216	1550	1552	1559	rVB2	36512	36674	1.04%	0.123%
20	11.327	1568	1571	1575	rBV	925185	847097	24.02%	2.838%
21	11.616	1617	1620	1623	rBV	57333	44682	1.27%	0.150%
22	11.716	1634	1637	1643	rVB	47232	43295	1.23%	0.145%
23	11.851	1657	1660	1664	rBV	103865	91563	2.60%	0.307%
24	12.022	1686	1689	1692	rVB2	48318	36503	1.04%	0.122%
25	12.410	1751	1755	1765	rVB4	43214	71033	2.01%	0.238%
26	12.733	1807	1810	1813	rBV2	54002	43414	1.23%	0.145%
27	12.921	1837	1842	1845	rBV	2699853	2552122	72.36%	8.551%
28	13.480	1933	1937	1940	rBV2	46196	51275	1.45%	0.172%
29	13.810	1989	1993	1996	rBV2	160440	189066	5.36%	0.633%
30	13.839	1996	1998	2005	rVB	235923	211762	6.00%	0.710%
31	13.945	2013	2016	2018	rBV	59248	54288	1.54%	0.182%
32	13.974	2018	2021	2030	rVB	840433	756451	21.45%	2.535%
33	14.133	2044	2048	2056	rVB	60662	71064	2.02%	0.238%
34	14.439	2097	2100	2105	rBV	74387	71346	2.02%	0.239%

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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

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35	14.598	2125	2127	2131	rVB	56604	48744	1.38%	0.163%
36	14.727	2145	2149	2157	rBV	615096	698130	19.80%	2.339%
37	14.815	2162	2164	2169	rVB2	34246	37051	1.05%	0.124%
38	15.074	2204	2208	2215	rVB	65434	82255	2.33%	0.276%
39	15.439	2264	2270	2281	rBV	503128	710596	20.15%	2.381%
40	15.880	2341	2345	2349	rVB	38763	53926	1.53%	0.181%
41	16.374	2425	2429	2436	rBV3	29482	49164	1.39%	0.165%

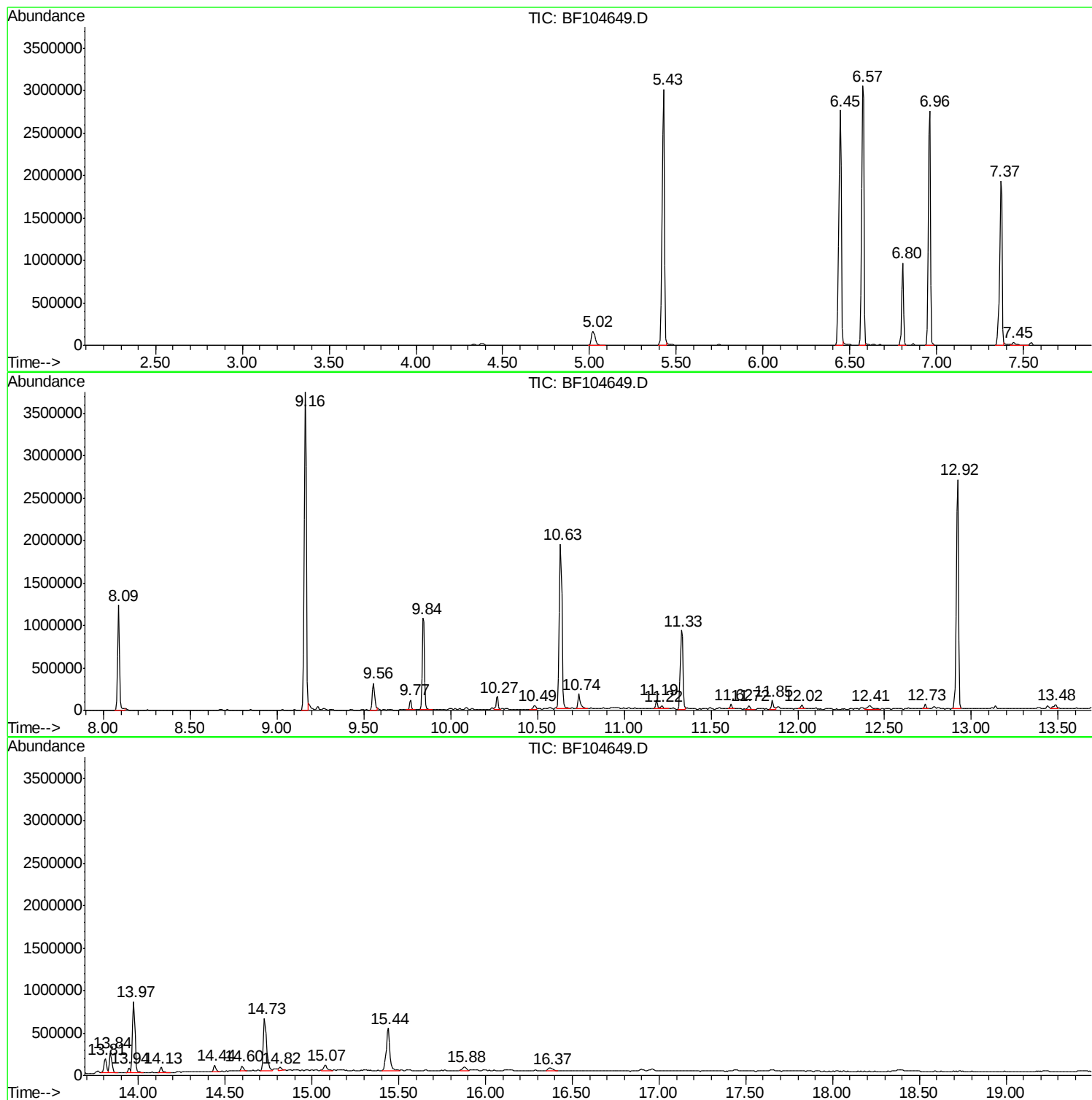
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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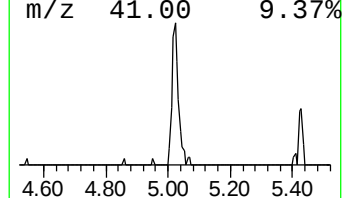
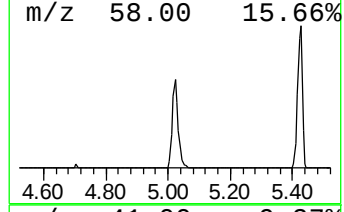
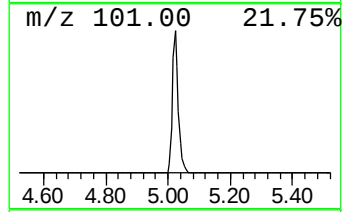
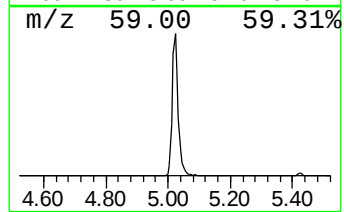
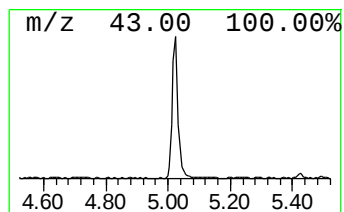
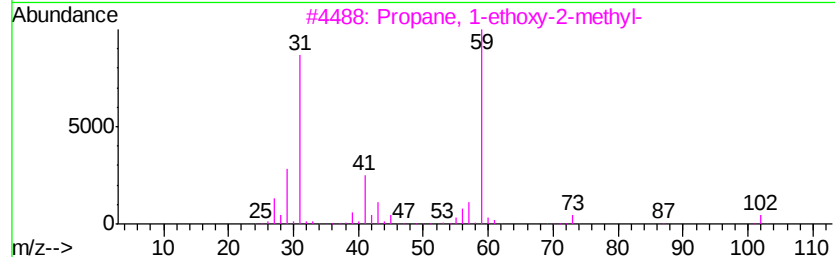
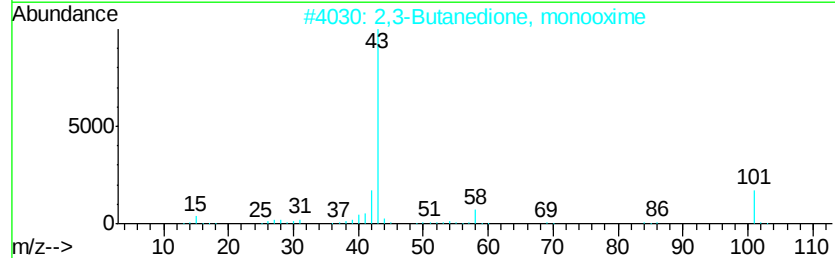
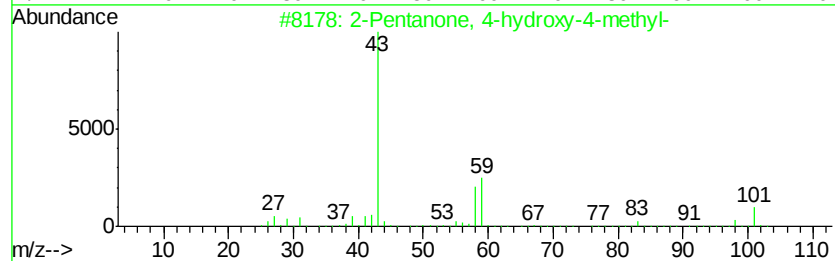
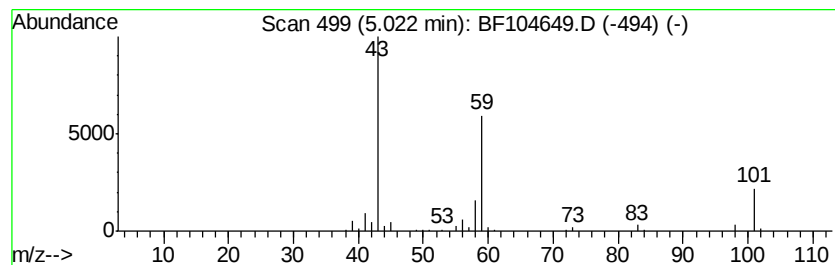
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	5.83 ng	222082	1,4-Dichlorobenzene-d4	6.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
4		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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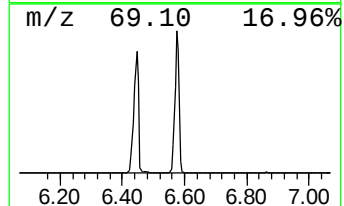
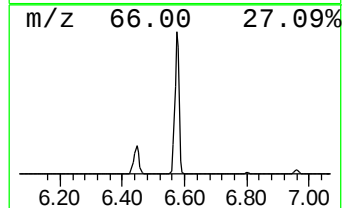
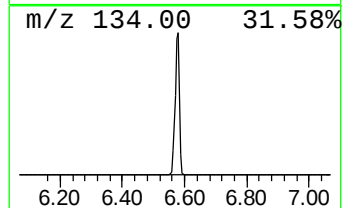
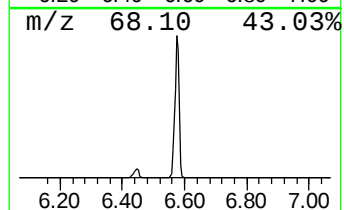
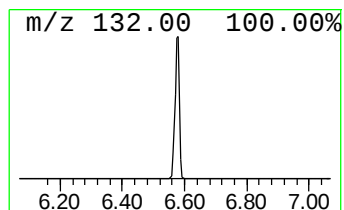
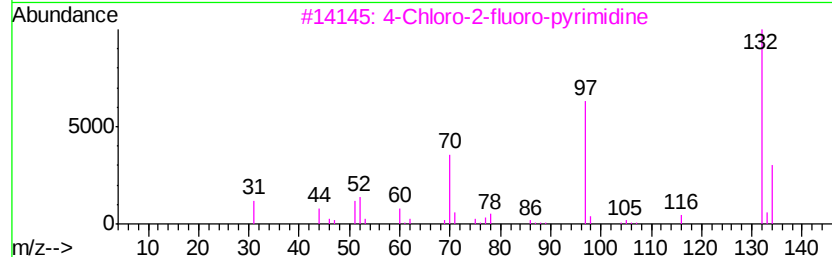
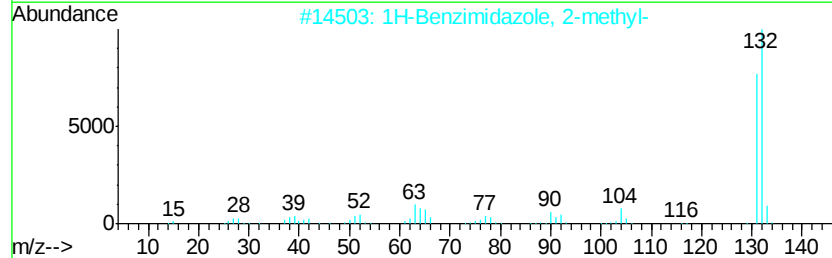
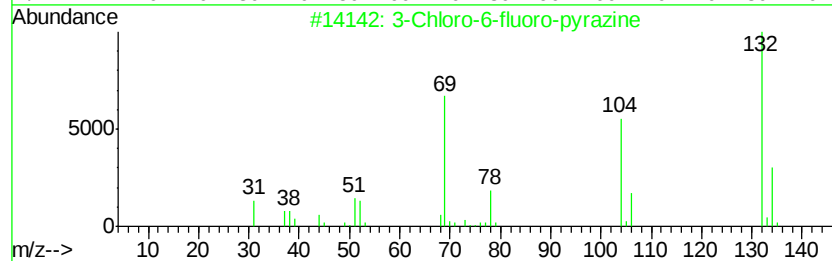
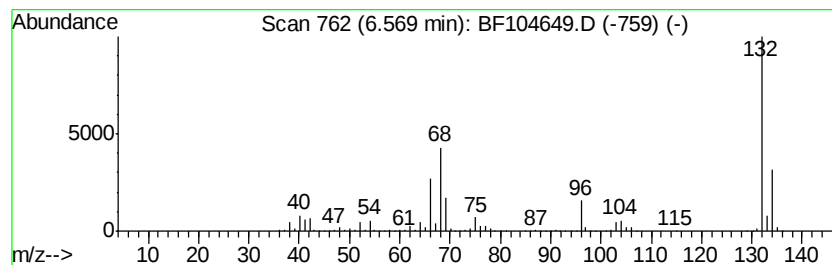
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	81.81 ng	3119040	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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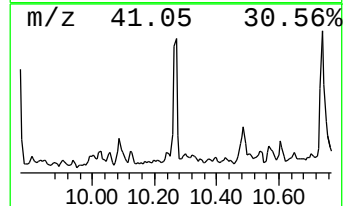
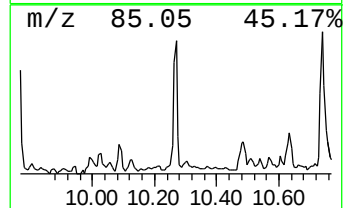
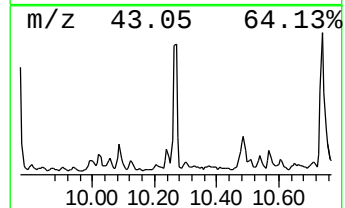
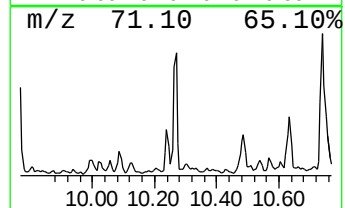
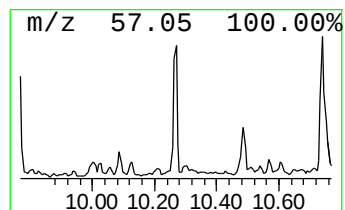
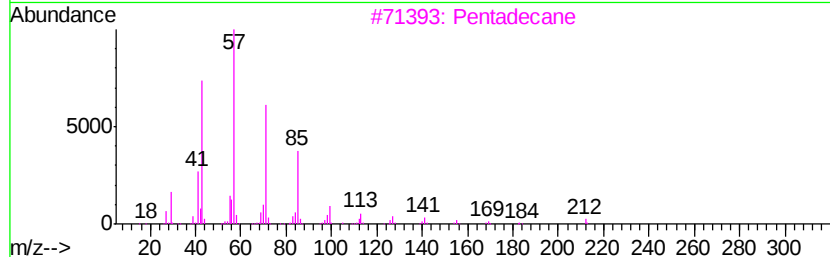
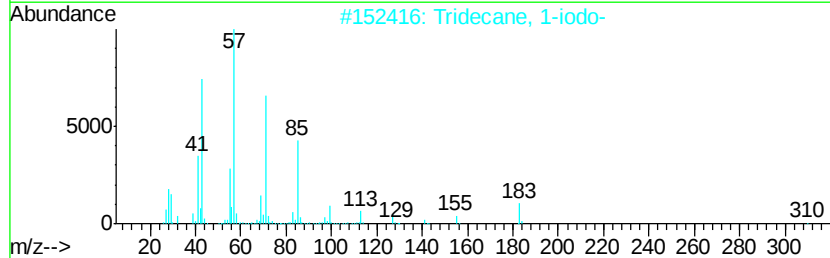
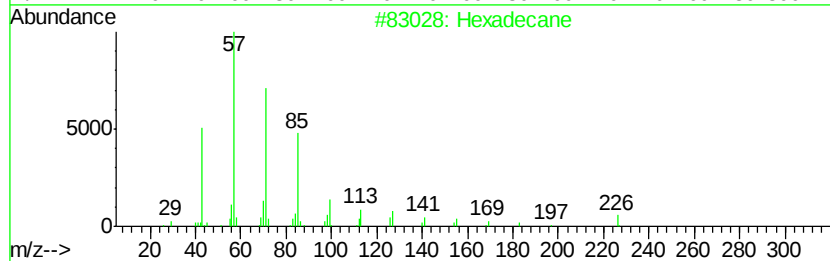
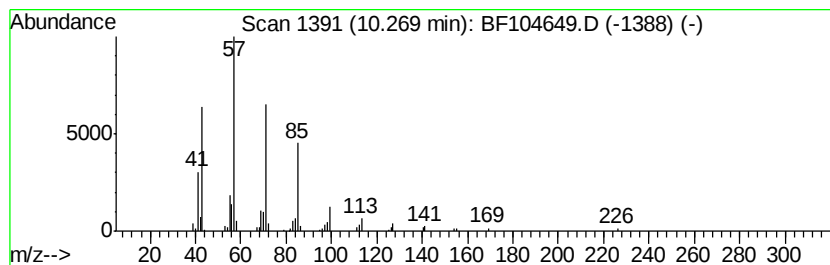
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.27	2.39 ng	124434	Acenaphthene-d10	9.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	97
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Tetradecane	198	C14H30	000629-59-4	87
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86



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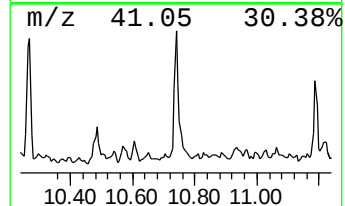
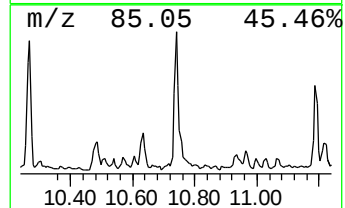
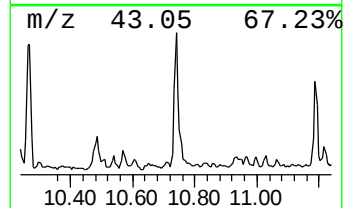
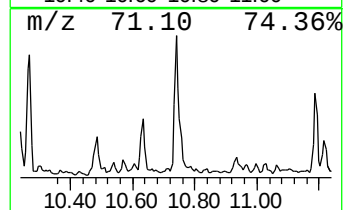
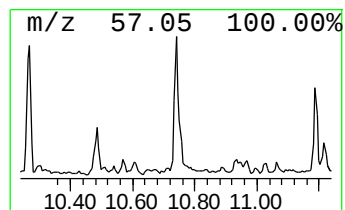
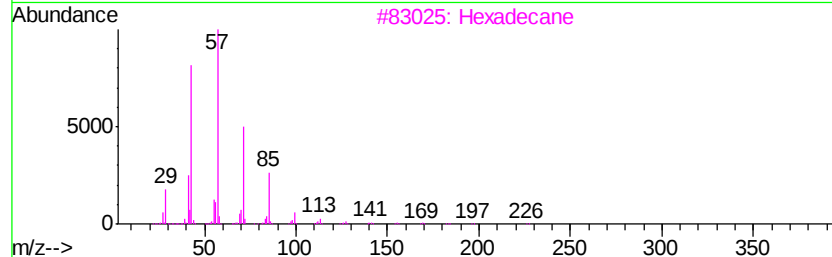
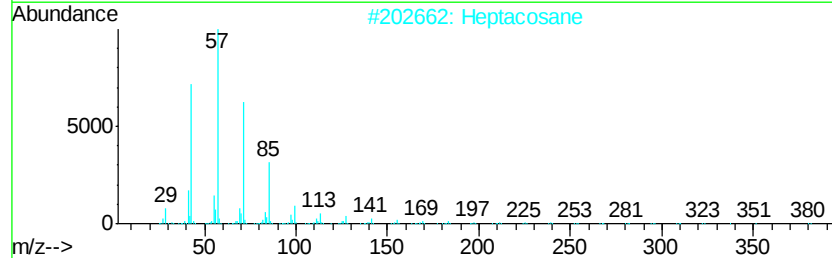
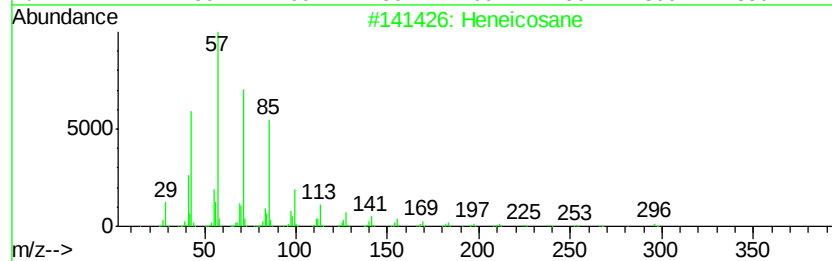
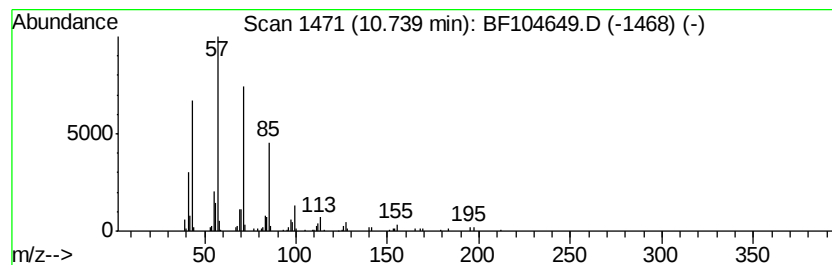
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Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	4.14 ng	175522	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heptacosane		380	C27H56	000593-49-7	91
3	Hexadecane		226	C16H34	000544-76-3	90
4	Tetracosane		338	C24H50	000646-31-1	90
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	87



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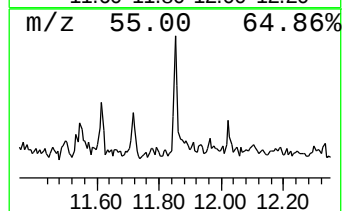
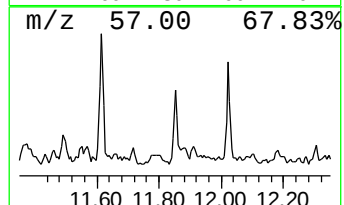
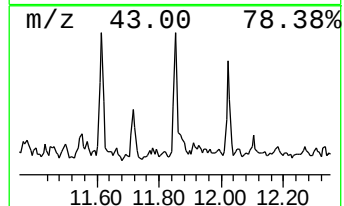
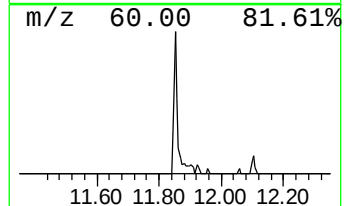
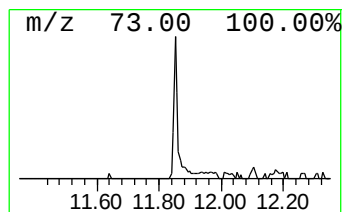
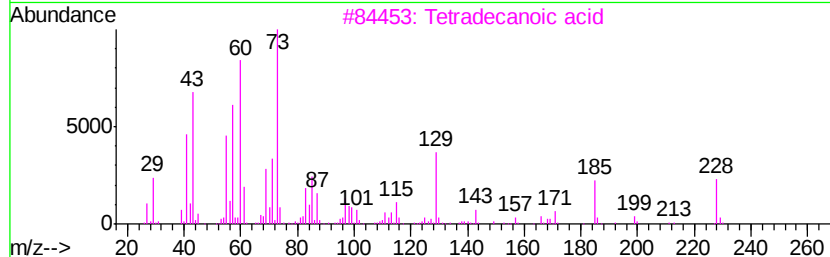
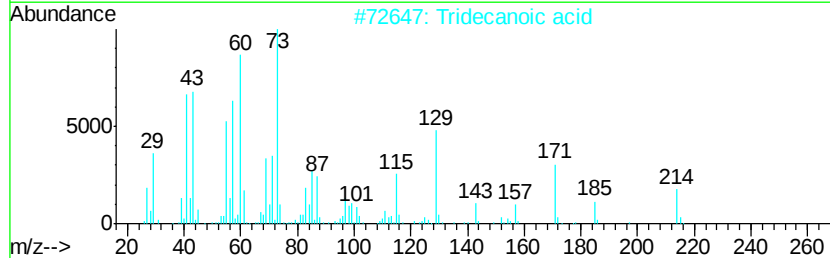
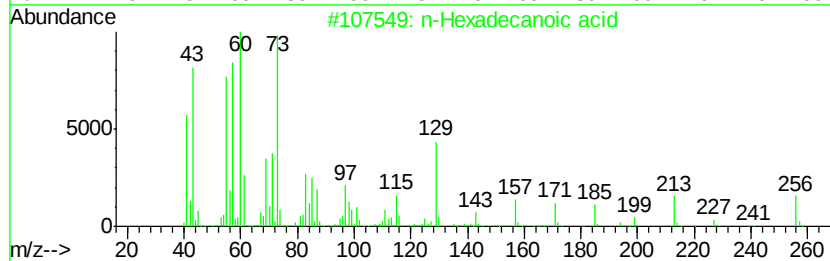
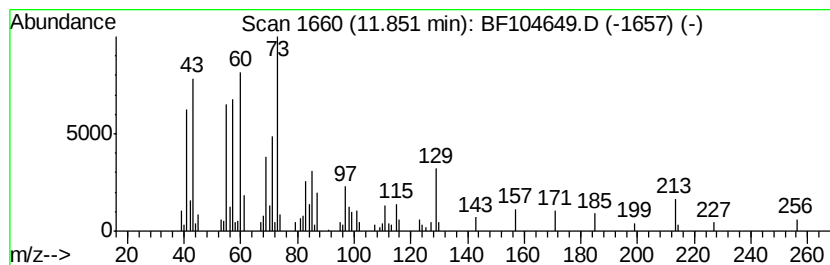
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.16 ng	91563	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	89
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041918\
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Acq On : 20 Apr 2018 00:42
Operator : JU/SJ
Sample : J2455-41
Misc :
ALS Vial : 19 Sample Multiplier: 1

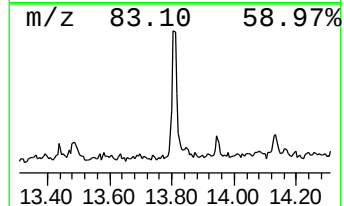
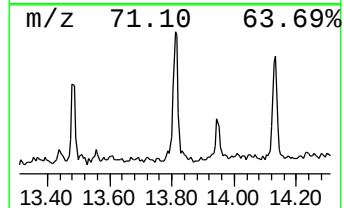
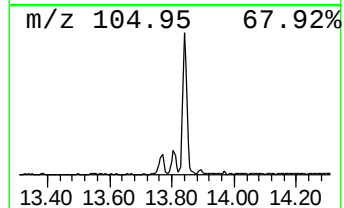
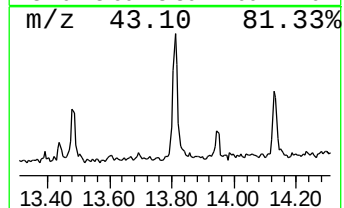
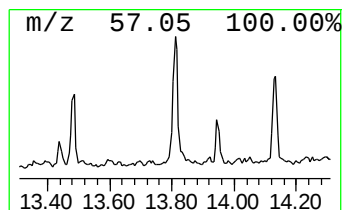
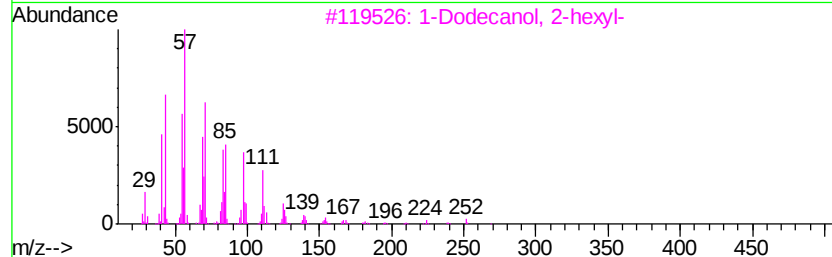
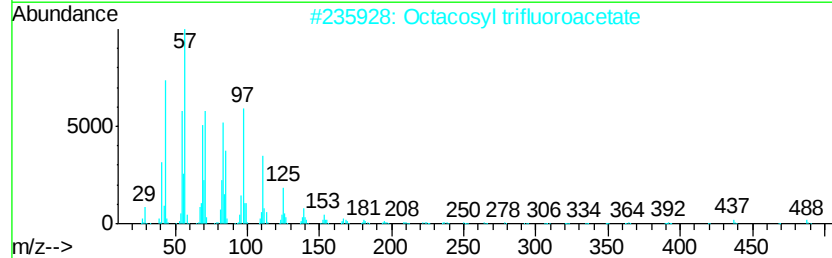
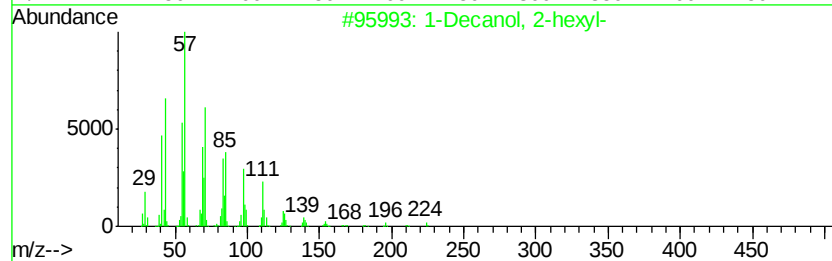
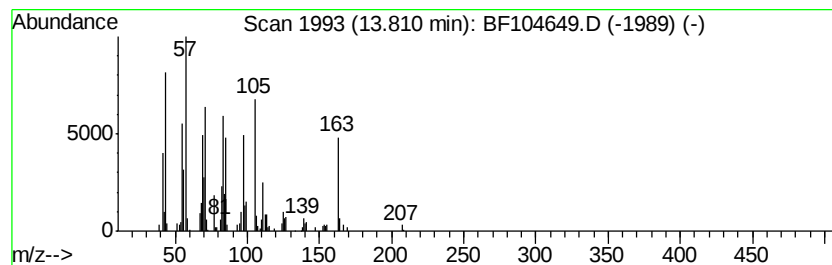
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ClientSampleId :
TP-1-BEDROCK

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Decanol, 2-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.81	5.00 ng	189066	Chrysene-d12	13.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	70
2		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	70
3		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	70
4		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	62
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	60



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Misc :
ALS Vial : 19 Sample Multiplier: 1

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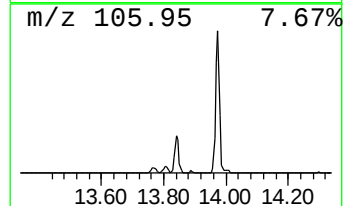
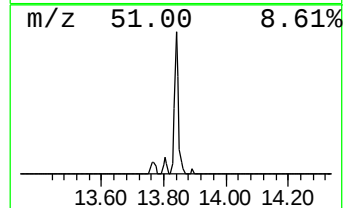
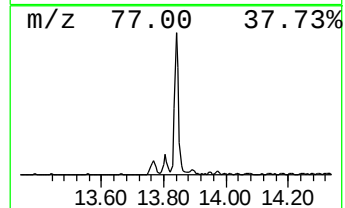
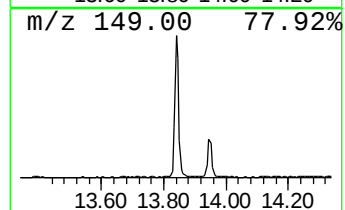
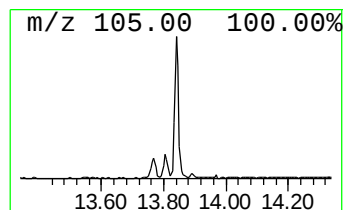
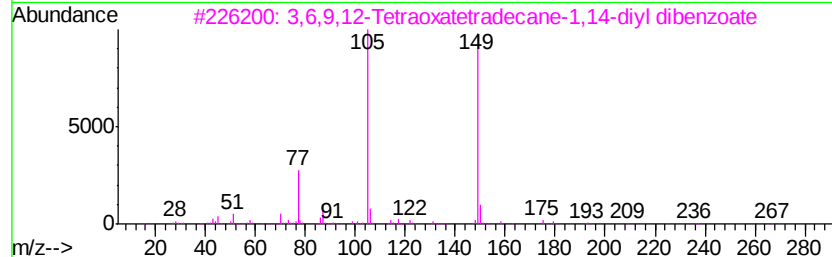
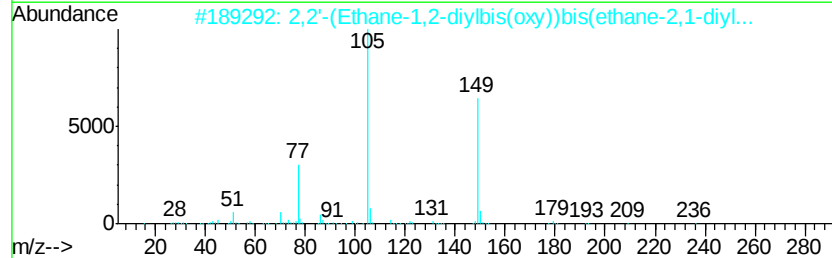
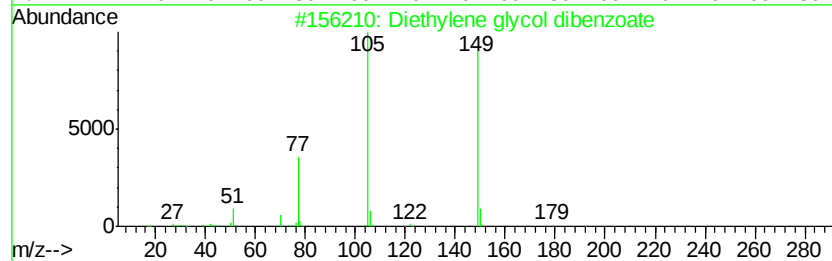
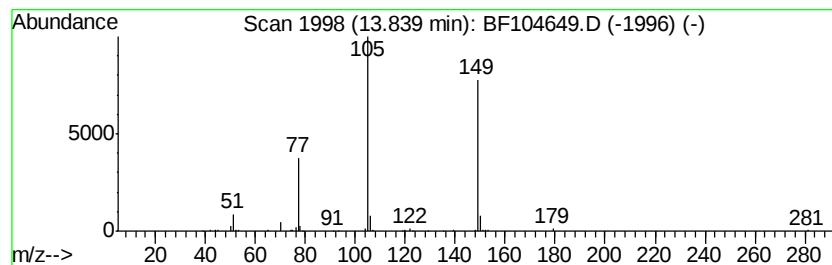
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	5.60 ng	211762	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2		2,2'-(Ethane-1,2-diylbis(oxv))bi...	358	C20H22O6	1000366-99-4	83
3		3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	78
4		Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
5		2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	64



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Sample : J2455-41
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-1-BEDROCK

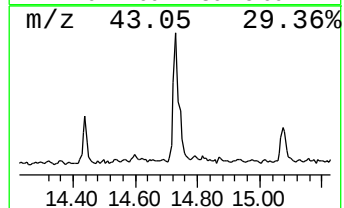
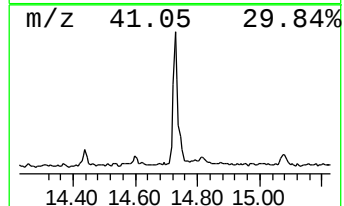
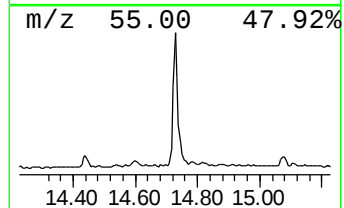
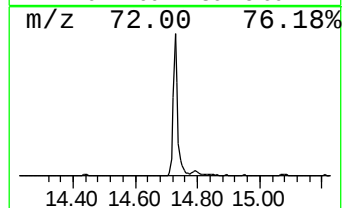
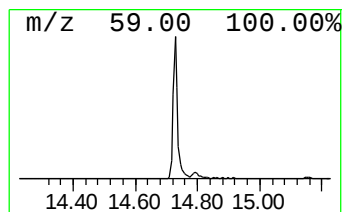
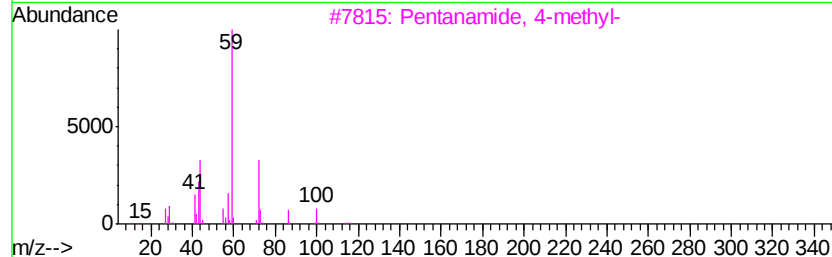
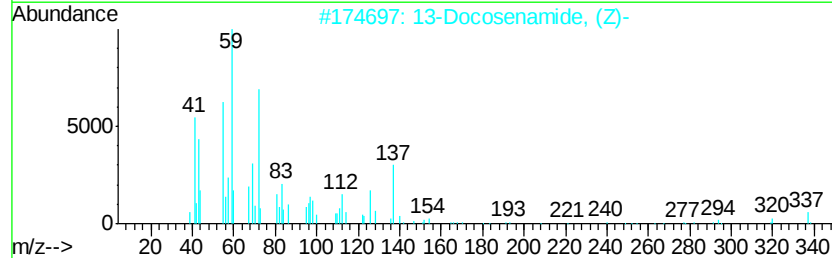
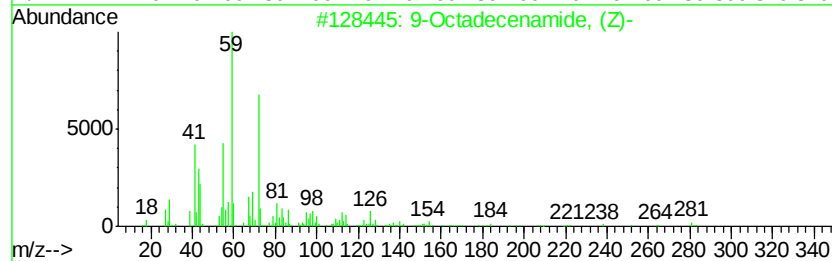
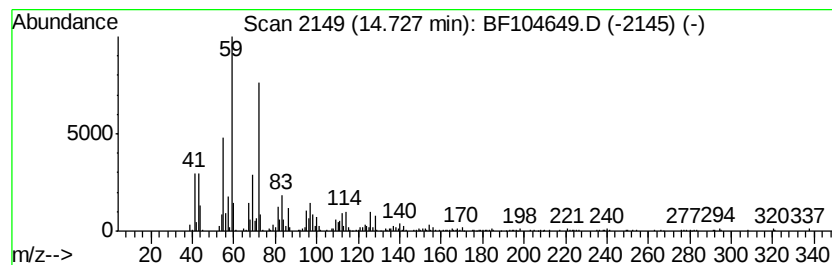
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	19.65 ng	698130	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	46
3		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	43
4		Hexadecanamide	255	C16H33NO	000629-54-9	43
5		Nonanamide	157	C9H19NO	001120-07-6	38



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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-1-BEDROCK

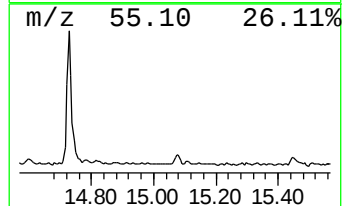
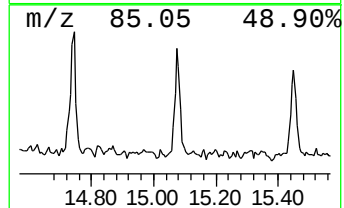
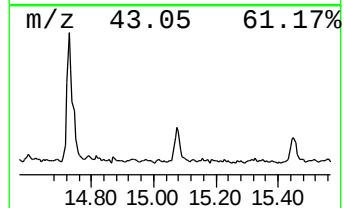
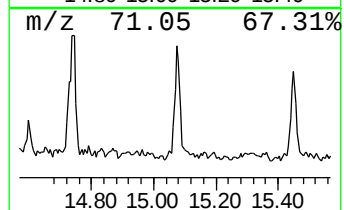
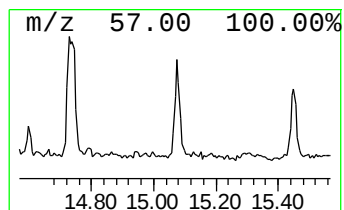
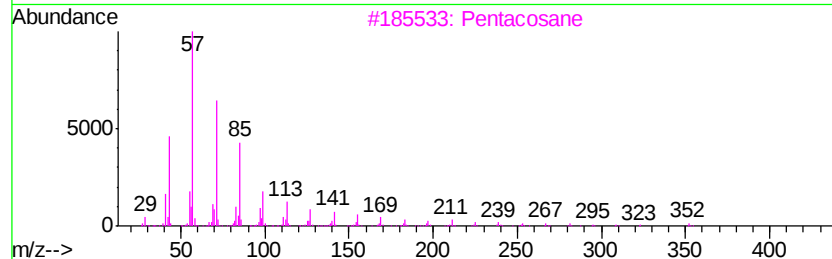
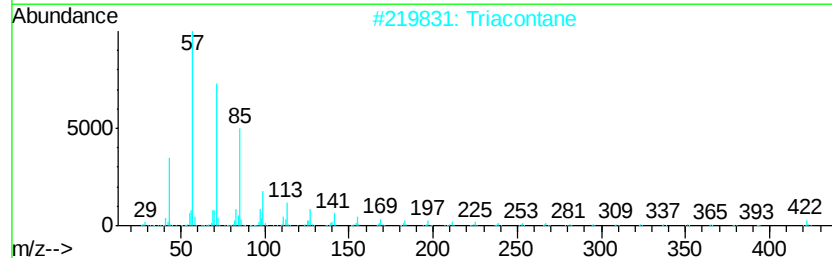
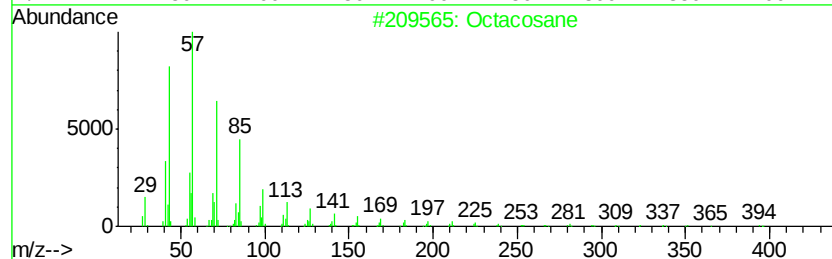
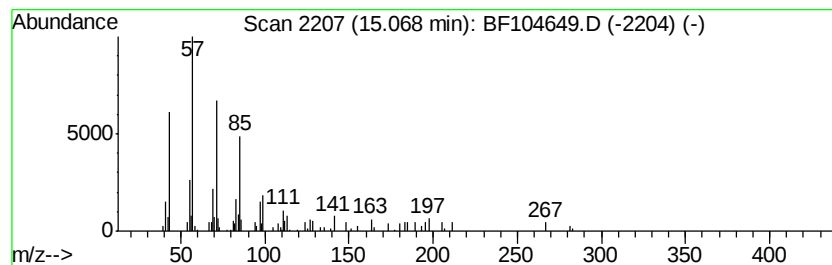
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.32 ng	82255	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		triacontane	422	C30H62	000638-68-6	91
3		Pentacosane	352	C25H52	000629-99-2	90
4		Heneicosane	296	C21H44	000629-94-7	87
5		Heptadecane	240	C17H36	000629-78-7	86



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Sample : J2455-41
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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
2-Pentanone, 4-hy...	5.02	5.8 ng		222082	1	6.80	762509	20.0
unknown6.57	6.57	81.8 ng		3119040	1	6.80	762509	20.0
Hexadecane	10.27	2.4 ng		124434	3	9.84	1041920	20.0
Heneicosane	10.74	4.1 ng		175522	4	11.33	847097	20.0
n-Hexadecanoic acid	11.85	2.2 ng		91563	4	11.33	847097	20.0
1-Decanol, 2-hexyl-	13.81	5.0 ng		189066	5	13.97	756451	20.0
Diethylene glycol...	13.84	5.6 ng		211762	5	13.97	756451	20.0
9-Octadecenamide,...	14.73	19.6 ng		698130	6	15.44	710596	20.0
Octacosane	15.07	2.3 ng		82255	6	15.44	710596	20.0