

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
 Data File : BF104526.D
 Acq On : 16 Apr 2018 11:40
 Operator : JU/SJ
 Sample : J2357-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR2520258

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	4.381	385	390	397	rBV	353921	407729	11.57%	1.113%
2	5.016	493	498	504	rBV	282066	365974	10.39%	0.999%
3	5.428	563	568	571	rBV	3045958	2971966	84.37%	8.116%
4	6.451	736	742	746	rBV	3189767	3440520	97.67%	9.395%
5	6.581	759	764	767	rBV	3537027	3288865	93.36%	8.981%
6	6.634	770	773	778	rVB2	55701	48881	1.39%	0.133%
7	6.810	799	803	806	rBV	1206275	1055049	29.95%	2.881%
8	6.863	809	812	817	rBV	62377	56935	1.62%	0.155%
9	6.963	825	829	832	rBV	3053282	2759788	78.34%	7.537%
10	7.375	891	899	902	rBV	2371183	2281563	64.77%	6.231%
11	7.451	908	912	915	rBV3	34061	41450	1.18%	0.113%
12	8.092	1017	1021	1024	rBV	1703737	1390511	39.47%	3.797%
13	9.169	1199	1204	1207	rBV	3903730	3522663	100.00%	9.620%
14	9.245	1214	1217	1219	rVB	45780	37616	1.07%	0.103%
15	9.563	1267	1271	1274	rBV	577511	534579	15.18%	1.460%
16	9.775	1301	1307	1310	rBV	158361	125784	3.57%	0.343%
17	9.845	1315	1319	1323	rBV	1574953	1472416	41.80%	4.021%
18	10.045	1349	1353	1358	rVB4	32277	53687	1.52%	0.147%
19	10.245	1384	1387	1389	rBV	44025	43798	1.24%	0.120%
20	10.275	1389	1392	1395	rVB	181569	136062	3.86%	0.372%
21	10.492	1425	1429	1432	rBV	38365	49426	1.40%	0.135%
22	10.639	1447	1454	1460	rBV	1460509	1460369	41.46%	3.988%
23	10.745	1470	1472	1482	rVB	135679	162029	4.60%	0.442%
24	10.939	1501	1505	1509	rBV4	30542	39723	1.13%	0.108%
25	11.198	1545	1549	1552	rBV	80836	77855	2.21%	0.213%
26	11.333	1569	1572	1575	rBV	1403884	1319958	37.47%	3.605%
27	11.357	1575	1576	1579	rVV	290271	191076	5.42%	0.522%
28	11.410	1583	1585	1588	rVB	59194	43438	1.23%	0.119%
29	11.557	1605	1610	1615	rBV3	78663	108372	3.08%	0.296%
30	11.627	1618	1622	1626	rBV2	45027	49584	1.41%	0.135%
31	11.839	1654	1658	1659	rBV	45586	43654	1.24%	0.119%
32	11.863	1659	1662	1667	rVV	312670	267224	7.59%	0.730%
33	11.951	1674	1677	1679	rBV	67575	70637	2.01%	0.193%
34	12.380	1747	1750	1754	rBV2	60790	81137	2.30%	0.222%

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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	12.551	1775	1779	1783	rVB	609235	517463	14.69%	1.413%
36	12.780	1812	1818	1821	rBV	540851	544997	15.47%	1.488%
37	12.804	1821	1822	1830	rVB2	81117	118587	3.37%	0.324%
38	12.927	1839	1843	1846	rVB	2851492	2606757	74.00%	7.119%
39	13.110	1871	1874	1876	rVB	67315	62796	1.78%	0.171%
40	13.174	1883	1885	1887	rVB	50582	38573	1.09%	0.105%
41	13.210	1887	1891	1895	rBV3	69838	92820	2.63%	0.253%
42	13.304	1904	1907	1910	rVB2	49506	46749	1.33%	0.128%
43	13.333	1910	1912	1916	rBV	43639	46969	1.33%	0.128%
44	13.492	1935	1939	1941	rBV4	29117	48409	1.37%	0.132%
45	13.616	1957	1960	1964	rVB	57135	64440	1.83%	0.176%
46	13.727	1974	1979	1982	rBV3	63625	101136	2.87%	0.276%
47	13.816	1991	1994	1998	rBV2	436681	447095	12.69%	1.221%
48	13.851	1998	2000	2005	rVB	82206	72475	2.06%	0.198%
49	13.980	2015	2022	2025	rBV2	1217329	1482999	42.10%	4.050%
50	14.004	2025	2026	2032	rVB	311418	242864	6.89%	0.663%
51	14.368	2084	2088	2091	rVB2	64089	94631	2.69%	0.258%
52	14.404	2092	2094	2098	rBV	37024	39609	1.12%	0.108%
53	14.839	2165	2168	2171	rVB2	137576	135644	3.85%	0.370%
54	15.021	2195	2199	2202	rBV	264256	386845	10.98%	1.056%
55	15.321	2247	2250	2256	rVB	155013	204428	5.80%	0.558%
56	15.386	2257	2261	2267	rVV	187921	247213	7.02%	0.675%
57	15.451	2267	2272	2281	rVV	693355	975019	27.68%	2.663%

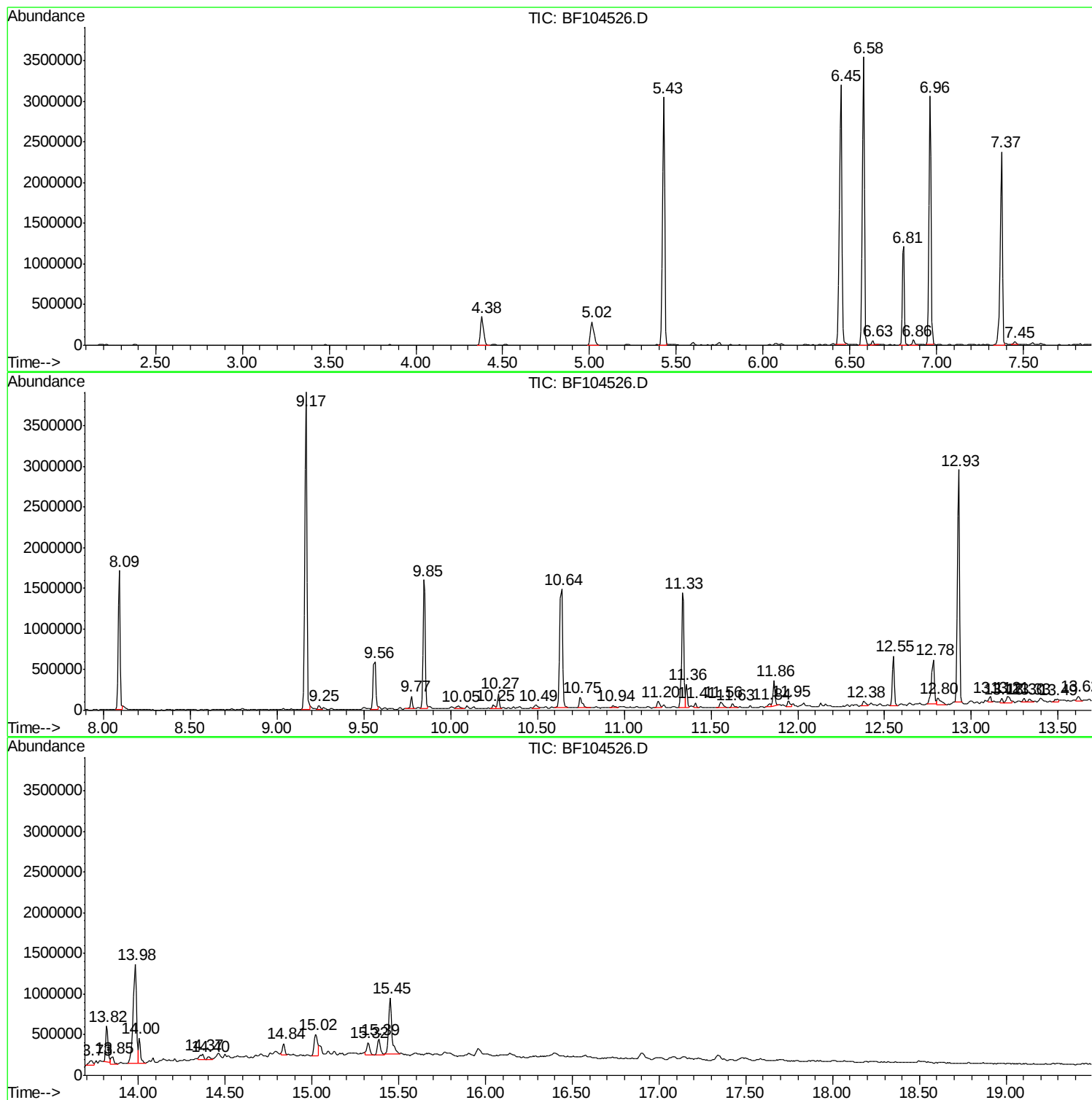
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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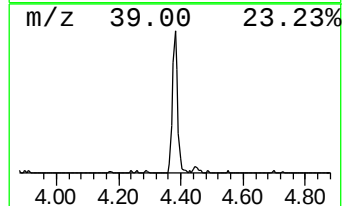
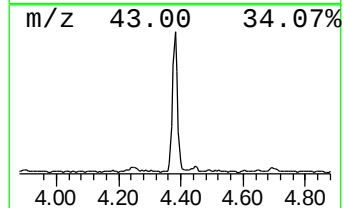
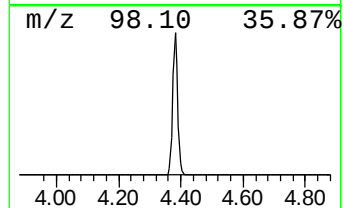
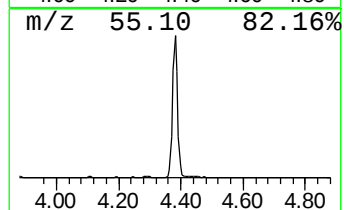
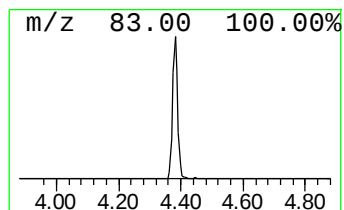
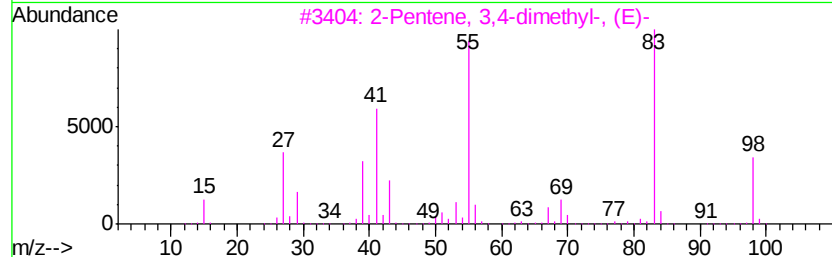
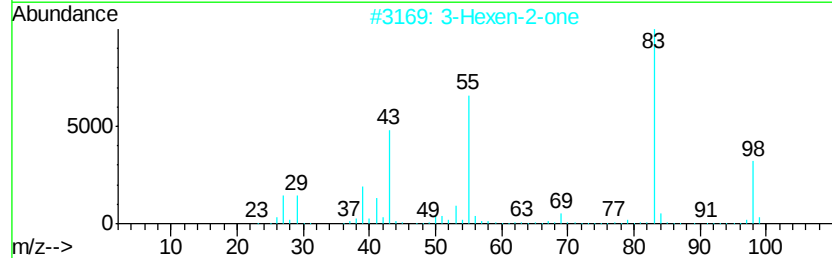
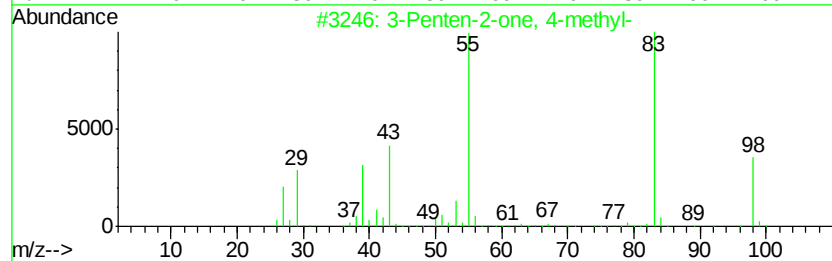
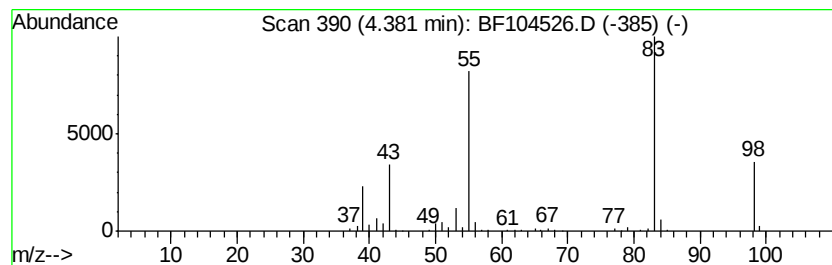
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.38	7.73 ng	407729	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78



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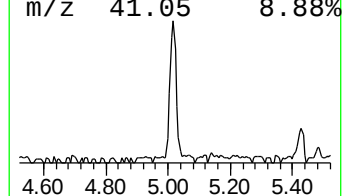
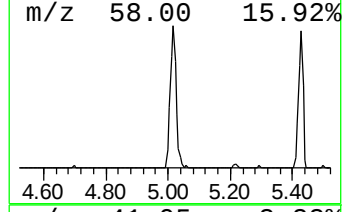
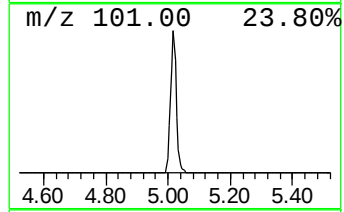
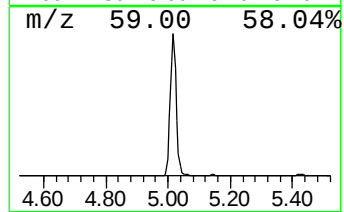
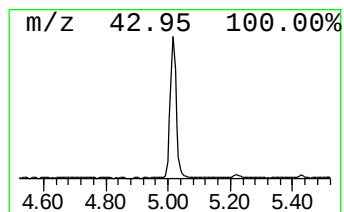
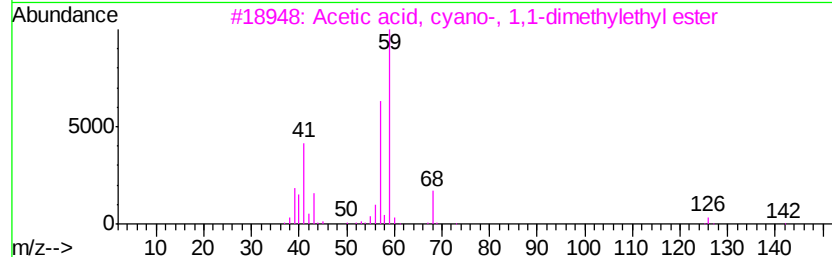
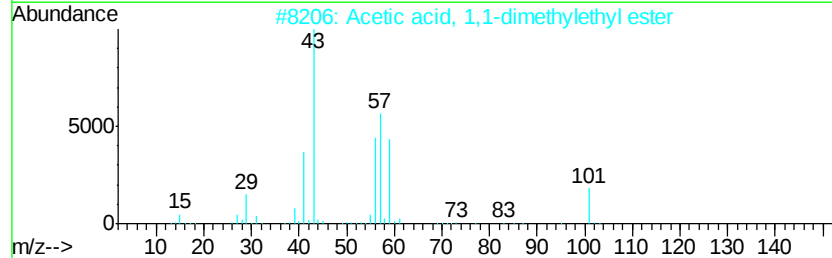
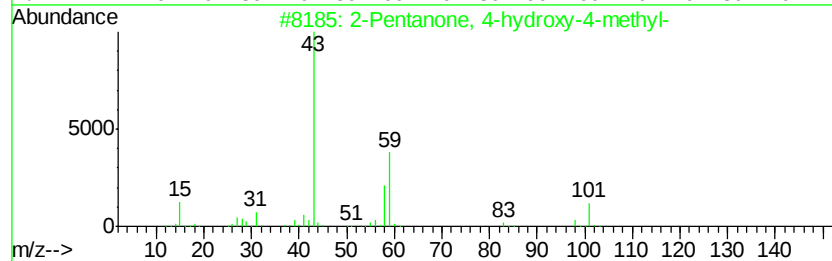
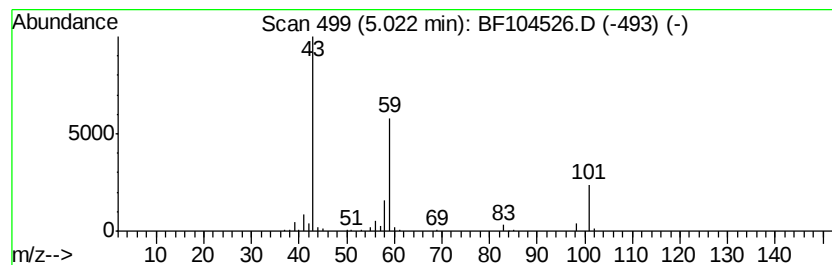
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	6.94 ng	365974	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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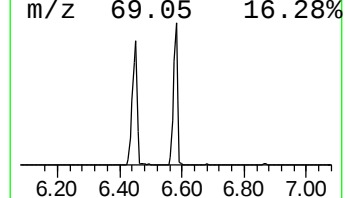
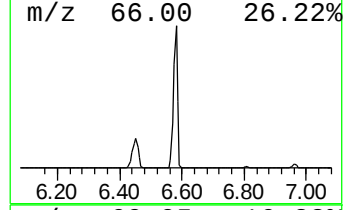
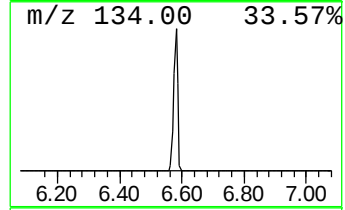
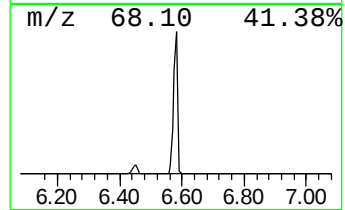
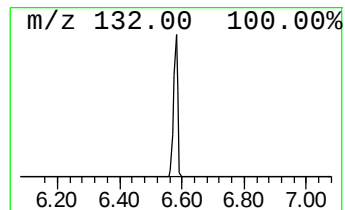
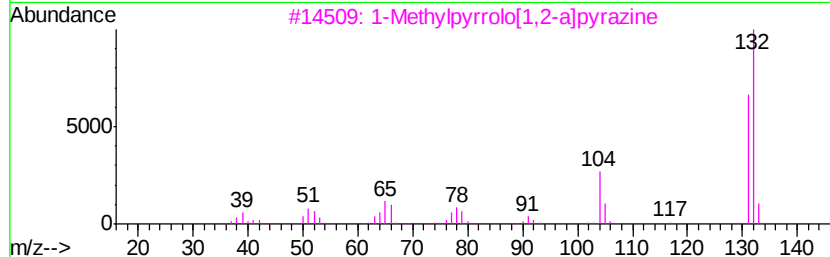
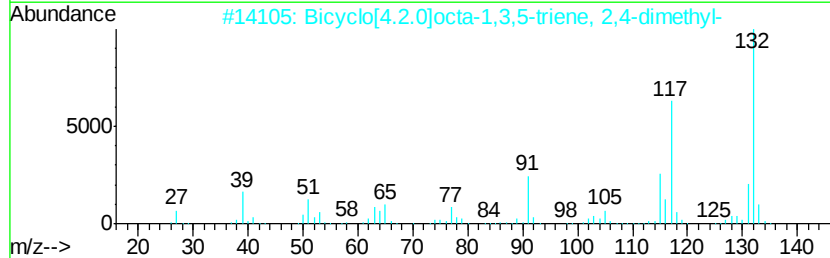
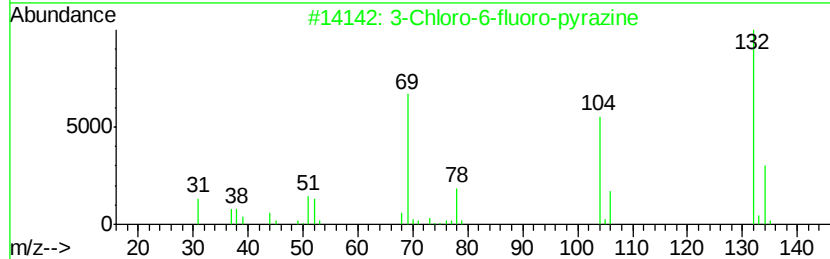
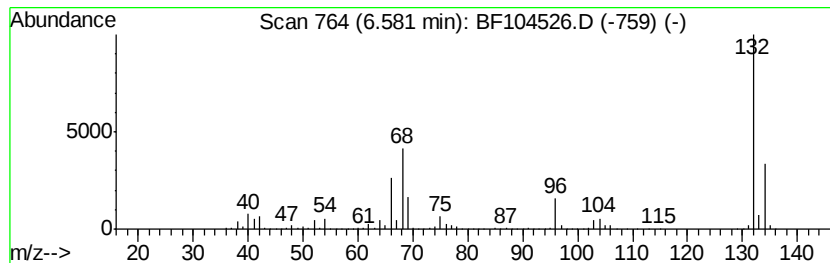
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	62.35 ng	3288870	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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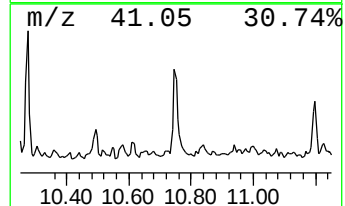
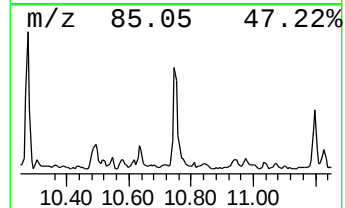
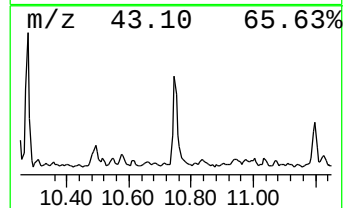
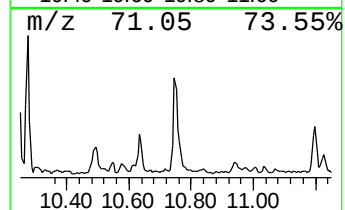
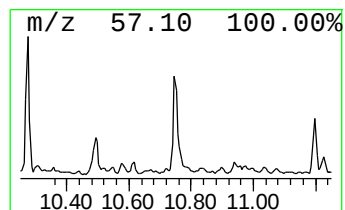
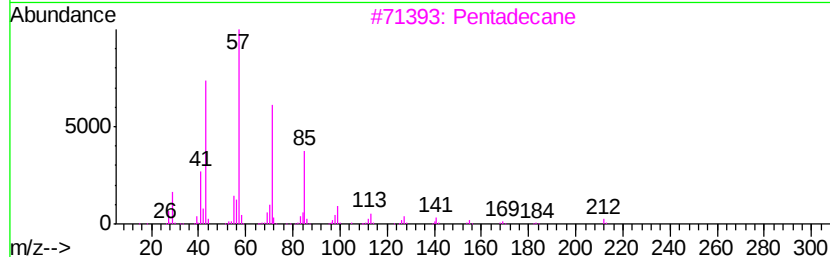
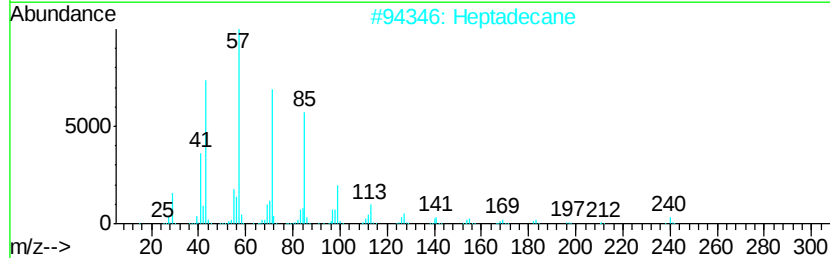
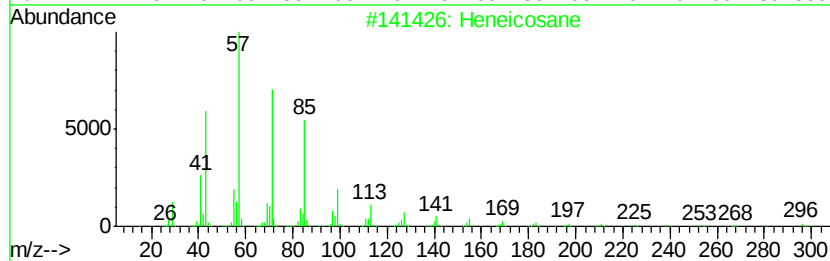
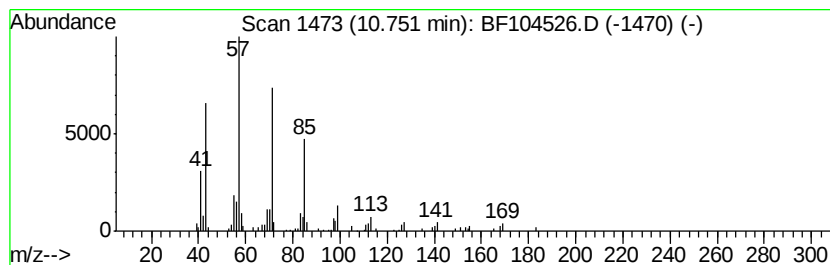
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.46 ng	162029	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heptadecane		240	C17H36	000629-78-7	91
3	Pentadecane		212	C15H32	000629-62-9	87
4	Eicosane		282	C20H42	000112-95-8	87
5	Hexadecane		226	C16H34	000544-76-3	86



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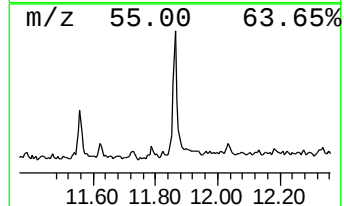
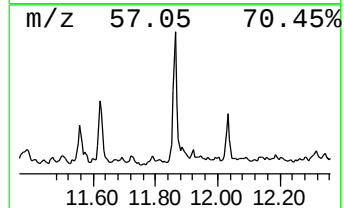
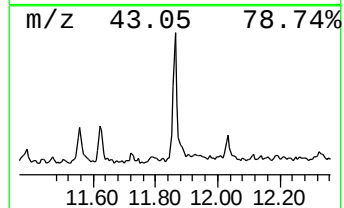
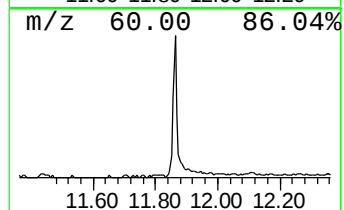
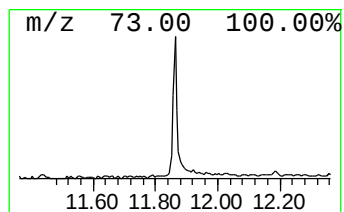
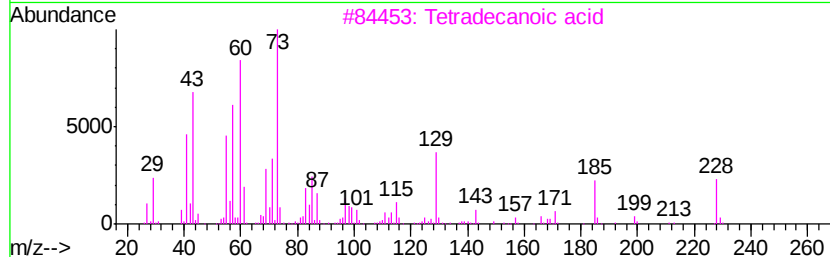
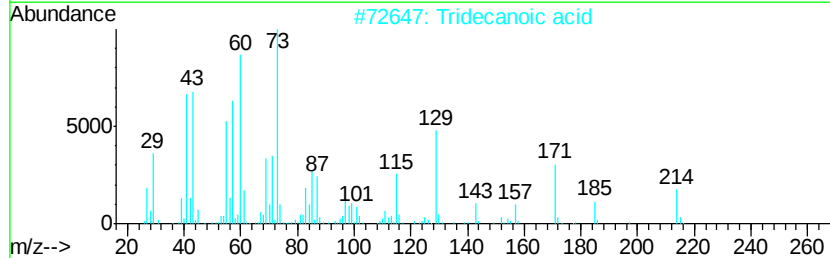
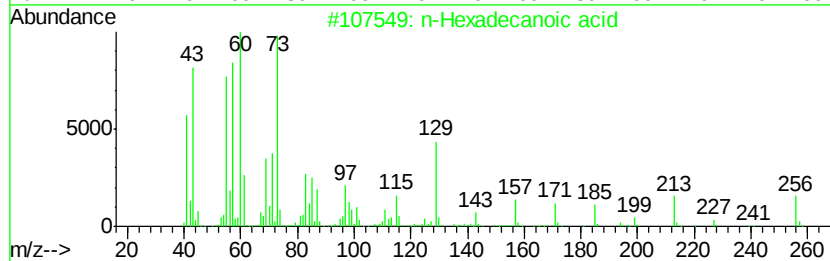
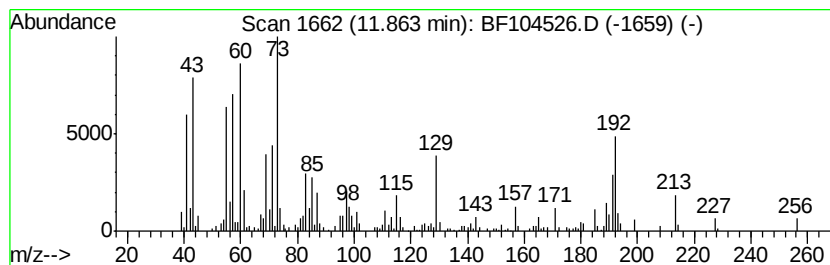
Instrument :
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ClientSampleId :
RBR2520258

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 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.86	4.05 ng	267224	Phenanthrene-d10	11.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041618\
Data File : BF104526.D
Acq On : 16 Apr 2018 11:40
Operator : JU/SJ
Sample : J2357-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

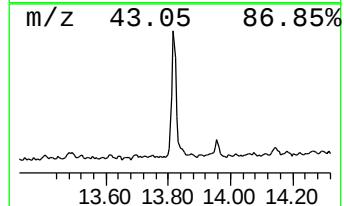
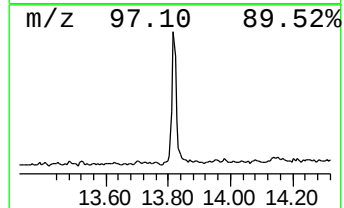
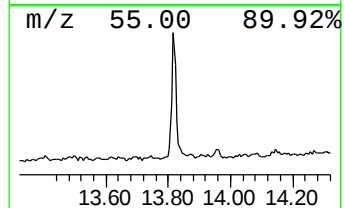
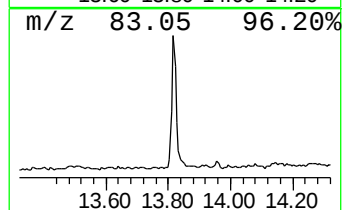
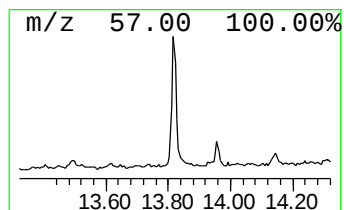
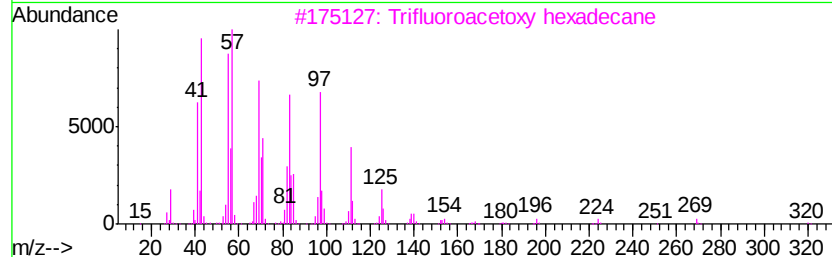
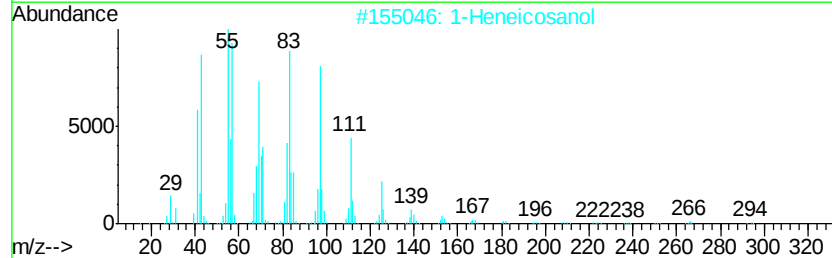
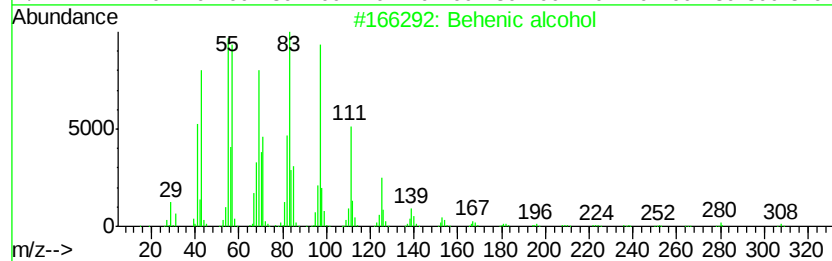
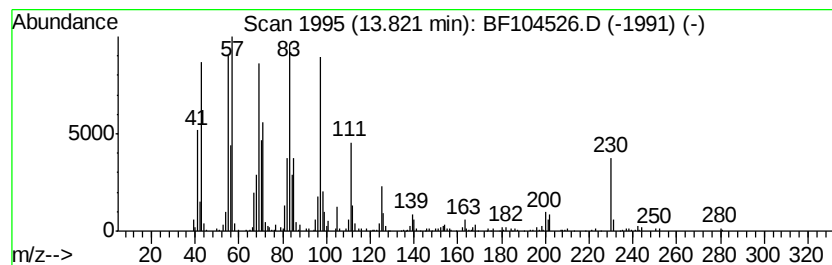
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.82	6.03 ng	447095	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	93
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041618\
Data File : BF104526.D
Acq On : 16 Apr 2018 11:40
Operator : JU/SJ
Sample : J2357-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

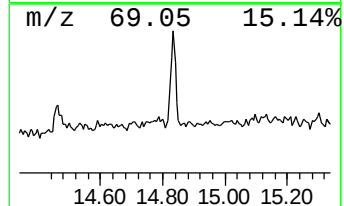
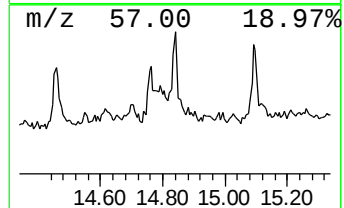
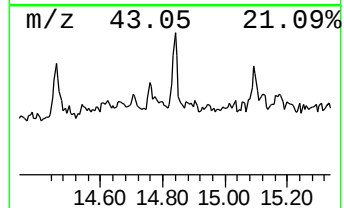
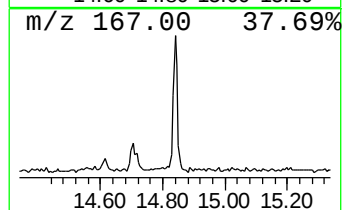
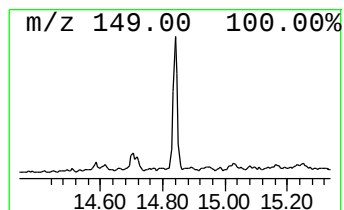
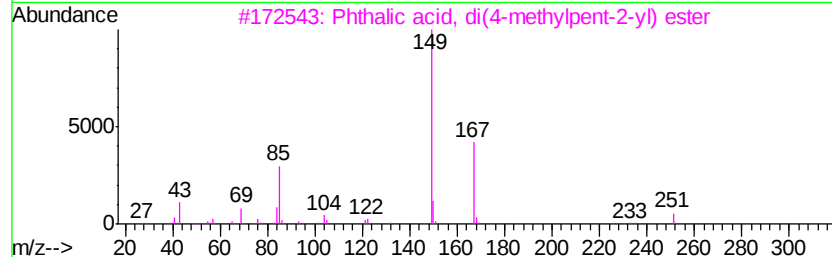
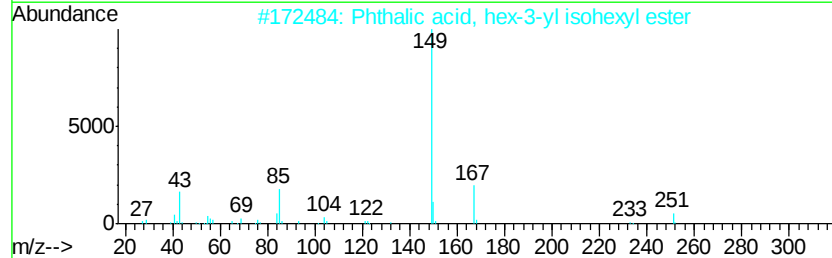
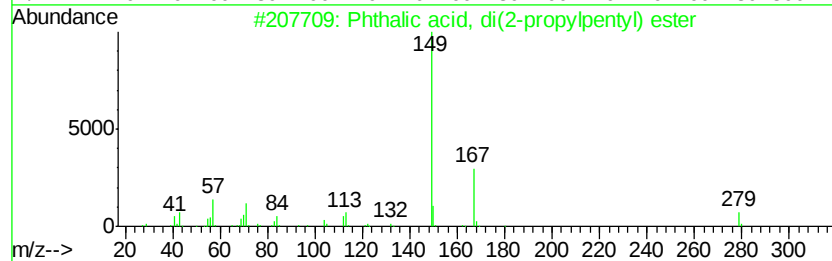
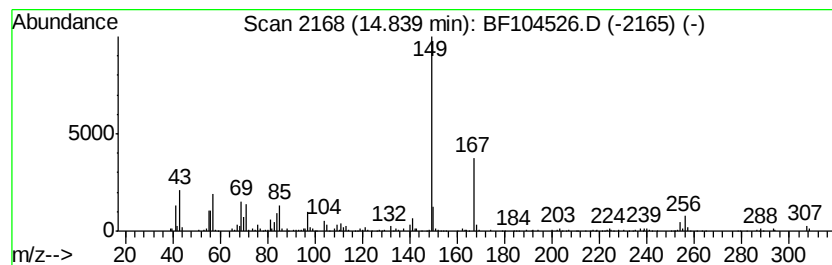
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phthalic acid, di(2-propylp... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.84	2.78 ng	135644	Perylene-d12	15.45		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, di(2-propylpentyl...	390	C24H38O4	1000377-93-5	64	
2	Phthalic acid, hex-3-yl isohexyl...	334	C20H30O4	1000356-95-6	59	
3	Phthalic acid, di(4-methylpent-2...	334	C20H30O4	1000356-88-6	59	
4	Phthalic acid, hexyl 4-methylpen...	334	C20H30O4	1000356-87-6	59	
5	Phthalic acid, di(hex-3-yl) ester	334	C20H30O4	1000356-96-7	59	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041618\
Data File : BF104526.D
Acq On : 16 Apr 2018 11:40
Operator : JU/SJ
Sample : J2357-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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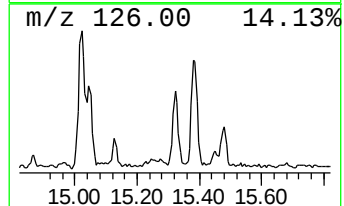
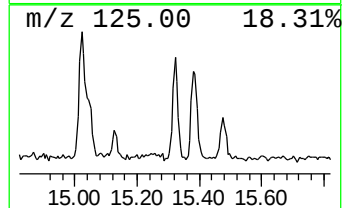
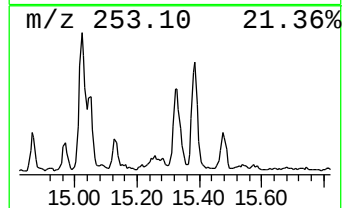
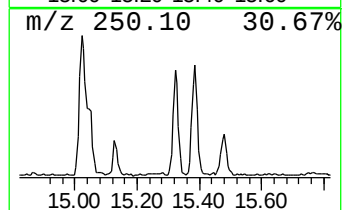
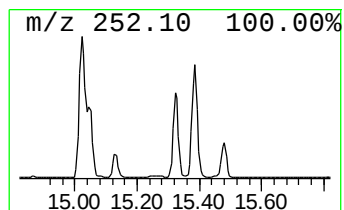
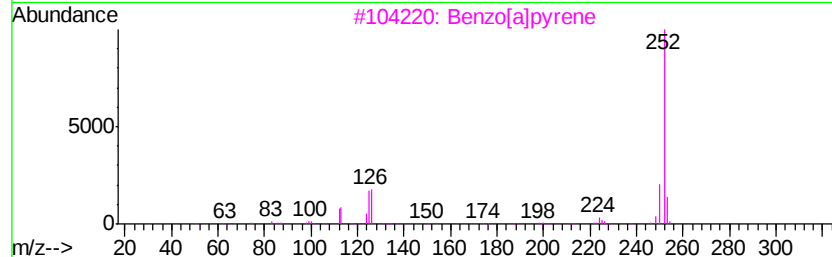
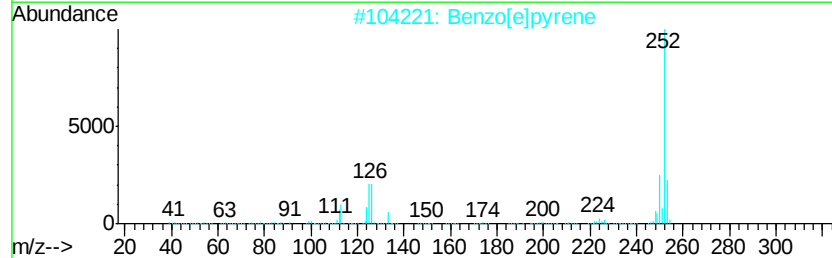
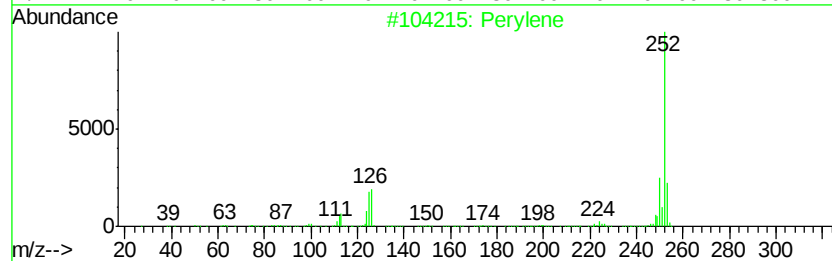
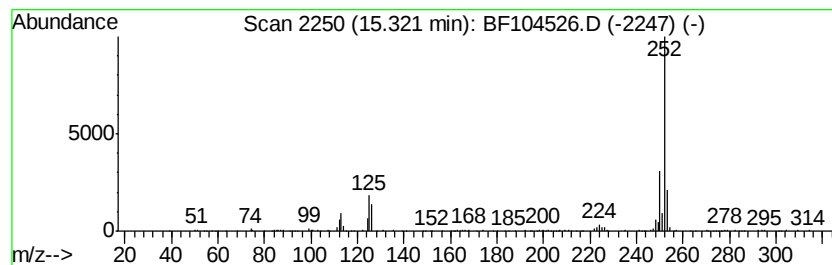
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Perylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	4.19 ng	204428	Perylene-d12	15.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	99
2		Benzo[e]pyrene	252	C20H12	000192-97-2	98
3		Benzo[a]pyrene	252	C20H12	000050-32-8	95
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	94
5		Benzo[j]fluoranthene	252	C20H12	000205-82-3	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041618\
Data File : BF104526.D
Acq On : 16 Apr 2018 11:40
Operator : JU/SJ
Sample : J2357-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR2520258

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
3-Penten-2-one, 4...	4.38	7.7	ng	407729	1	6.81	1055050	20.0
2-Pentanone, 4-hy...	5.02	6.9	ng	365974	1	6.81	1055050	20.0
unknown6.58	6.58	62.4	ng	3288870	1	6.81	1055050	20.0
Heneicosane	10.75	2.5	ng	162029	4	11.33	1319960	20.0
n-Hexadecanoic acid	11.86	4.0	ng	267224	4	11.33	1319960	20.0
Behenic alcohol	13.82	6.0	ng	447095	5	13.98	1483000	20.0
Phthalic acid, di...	14.84	2.8	ng	135644	6	15.45	975019	20.0
Perylene	15.32	4.2	ng	204428	6	15.45	975019	20.0