

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
 Data File : BF112504.D
 Acq On : 12 Feb 2019 11:26
 Operator : JU/SJ
 Sample : K1442-05
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-11

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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	5.051	501	504	516	rBV	87422	125759	4.25%	0.417%
2	5.469	571	575	597	rBV	2503997	2569667	86.84%	8.515%
3	6.487	744	748	765	rBV	2646444	2762398	93.35%	9.153%
4	6.610	765	769	776	rVV	3254238	2876987	97.22%	9.533%
5	6.834	803	807	815	rBV	856609	748070	25.28%	2.479%
6	6.992	829	834	837	rBV	2348850	2219091	74.99%	7.353%
7	7.398	899	903	914	rBV	1807949	1686216	56.98%	5.587%
8	8.116	1021	1025	1040	rVB	1018311	944533	31.92%	3.130%
9	9.186	1203	1207	1217	rBV	3205497	2959143	100.00%	9.805%
10	9.580	1271	1274	1283	rVB	205156	192972	6.52%	0.639%
11	9.733	1297	1300	1306	rBV	41868	39442	1.33%	0.131%
12	9.869	1313	1323	1327	rBV	1034608	976259	32.99%	3.235%
13	9.904	1327	1329	1335	rVB	38137	42197	1.43%	0.140%
14	10.663	1454	1458	1468	rBV	1680564	1648987	55.73%	5.464%
15	10.839	1485	1488	1490	rBV	36580	32919	1.11%	0.109%
16	11.210	1548	1551	1554	rBV2	87548	81065	2.74%	0.269%
17	11.304	1564	1567	1572	rBV7	21672	31719	1.07%	0.105%
18	11.357	1573	1576	1579	rVV	901186	829539	28.03%	2.749%
19	11.380	1579	1580	1587	rVV	269367	219486	7.42%	0.727%
20	11.433	1587	1589	1592	rVV	51841	48246	1.63%	0.160%
21	11.598	1614	1617	1622	rBV3	30089	37409	1.26%	0.124%
22	11.639	1622	1624	1628	rVB2	33591	35813	1.21%	0.119%
23	11.880	1659	1665	1673	rBV3	419745	563784	19.05%	1.868%
24	11.974	1678	1681	1683	rBV	91797	85825	2.90%	0.284%
25	12.045	1690	1693	1696	rBV	90081	82310	2.78%	0.273%
26	12.151	1709	1711	1714	rVB	37608	32400	1.09%	0.107%
27	12.298	1732	1736	1739	rBV4	45802	67247	2.27%	0.223%
28	12.410	1753	1755	1757	rBV	43887	37282	1.26%	0.124%
29	12.574	1780	1783	1787	rBV	612561	553191	18.69%	1.833%
30	12.663	1795	1798	1804	rBV2	299169	337596	11.41%	1.119%
31	12.804	1816	1822	1825	rBV	613167	623931	21.08%	2.067%
32	12.939	1841	1845	1848	rBV	2477682	2105609	71.16%	6.977%
33	13.833	1994	1997	2000	rBV2	226706	187440	6.33%	0.621%
34	14.004	2022	2026	2029	rBV2	816987	1036496	35.03%	3.434%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.033	2029	2031	2034	rVB	266245	222028	7.50%	0.736%
36	14.145	2048	2050	2054	rBV2	159364	171871	5.81%	0.570%
37	14.451	2100	2102	2108	rBV	210007	230119	7.78%	0.763%
38	14.574	2121	2123	2129	rBV	353725	362744	12.26%	1.202%
39	14.757	2151	2154	2157	rVB	334351	306319	10.35%	1.015%
40	15.092	2208	2211	2214	rVB2	515847	565497	19.11%	1.874%
41	15.468	2272	2275	2282	rVB2	459510	928246	31.37%	3.076%
42	15.898	2345	2348	2353	rVB2	415634	571178	19.30%	1.893%

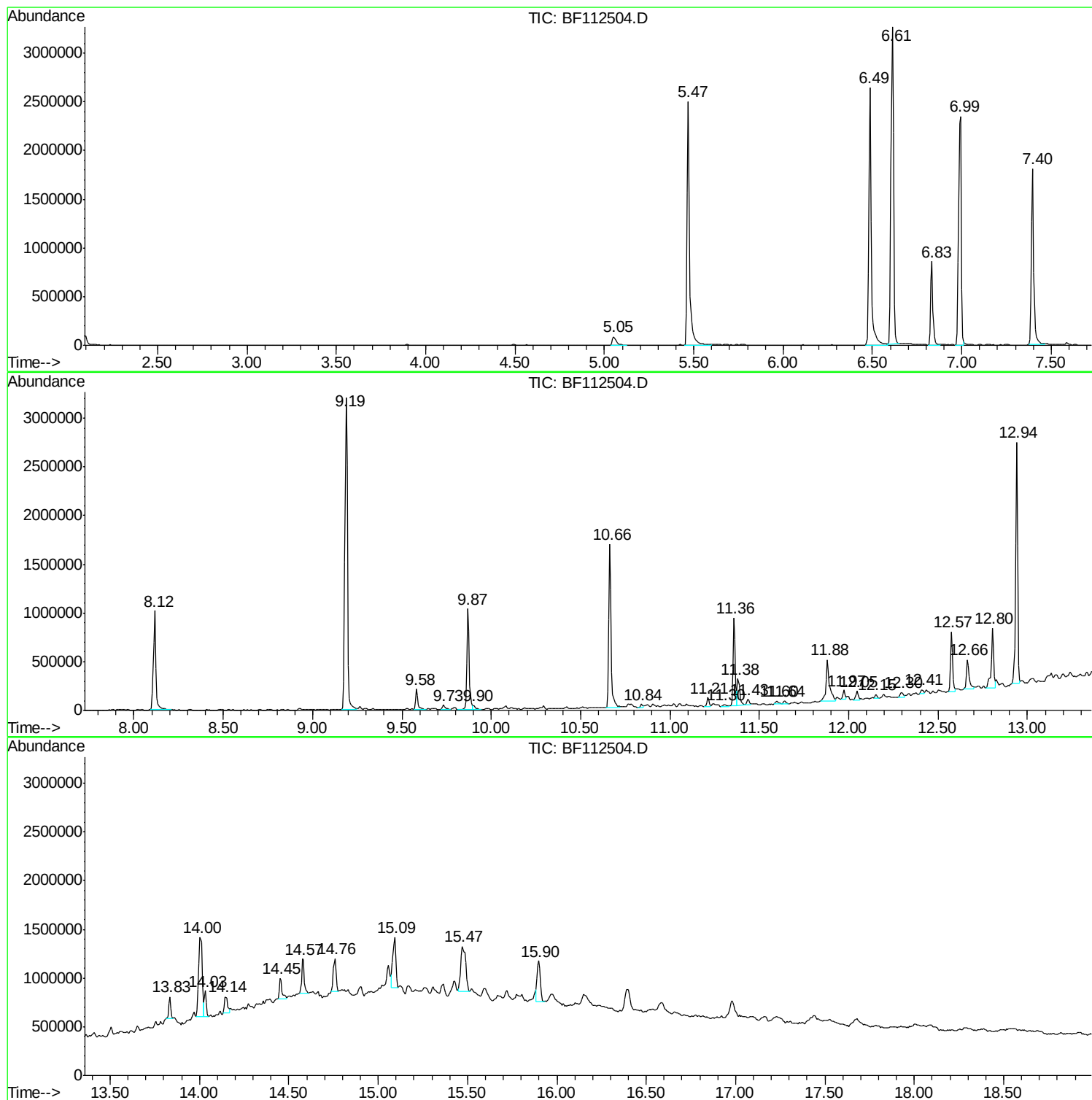
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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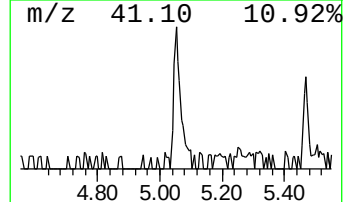
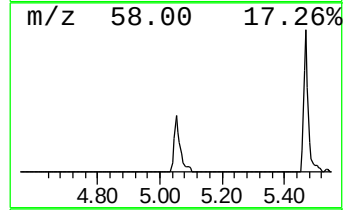
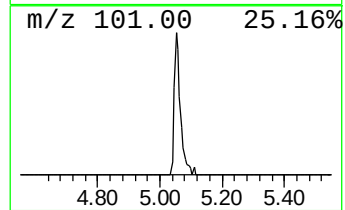
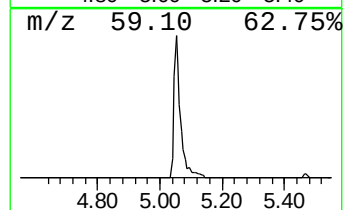
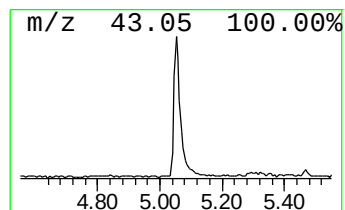
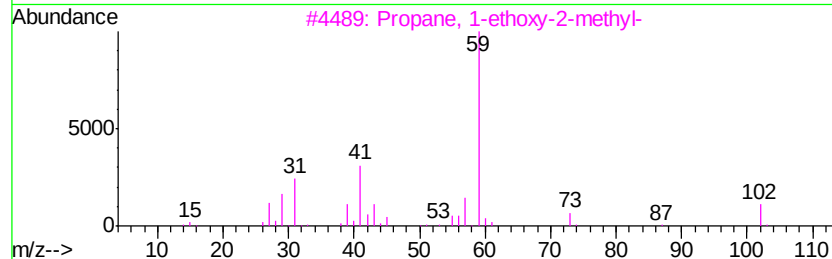
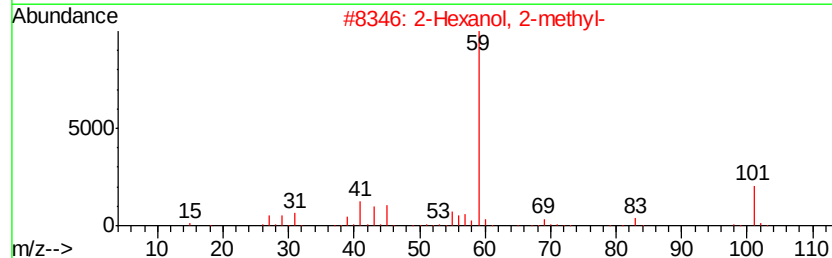
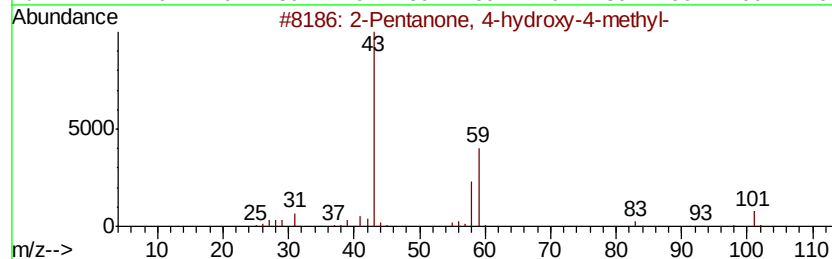
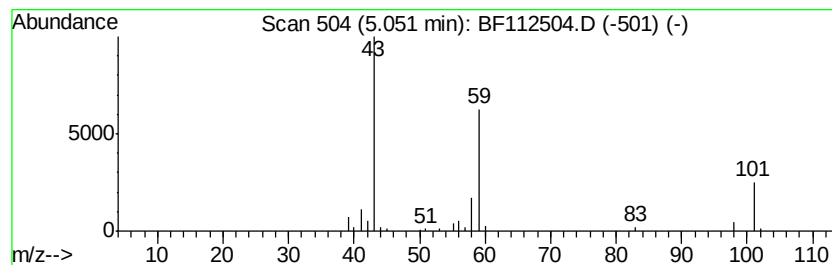
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	3.36 ng	125759	1,4-Dichlorobenzene-d4	6.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25	
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	23	
4	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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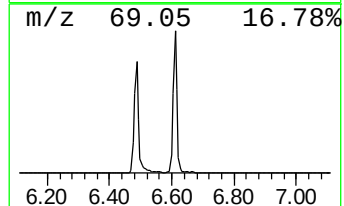
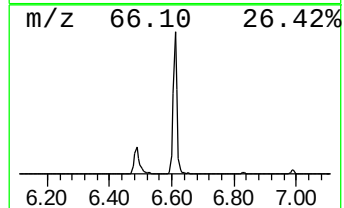
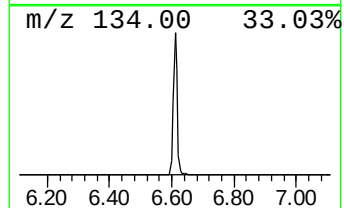
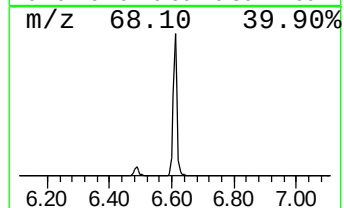
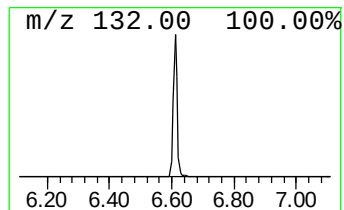
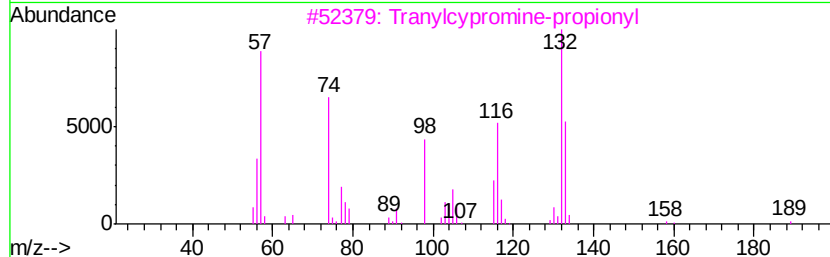
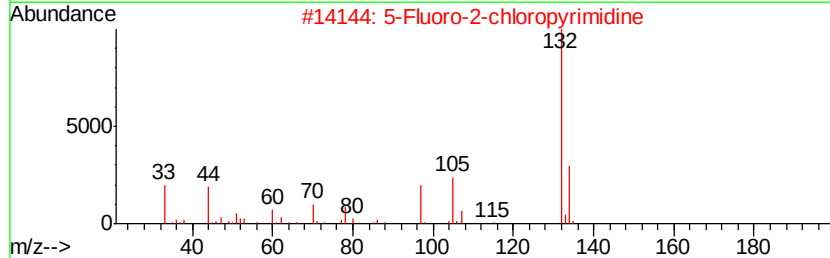
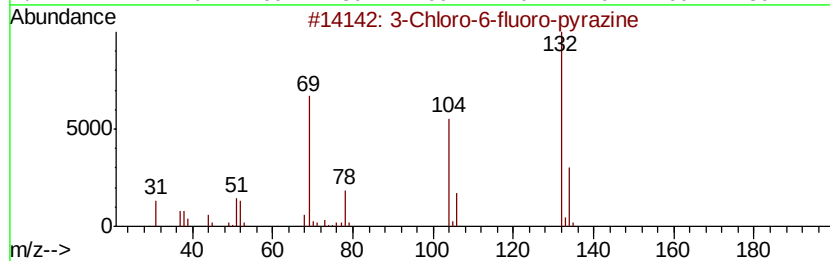
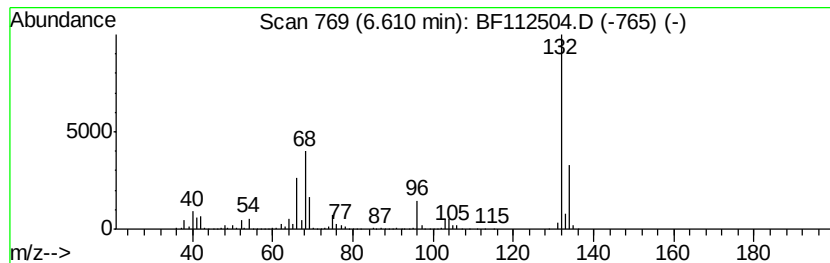
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Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	76.92 ng	2876990	1,4-Dichlorobenzene-d4	6.83

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		Tranvlcypramine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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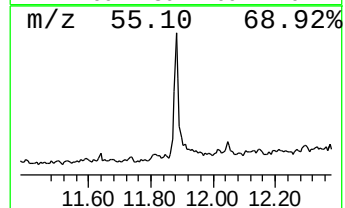
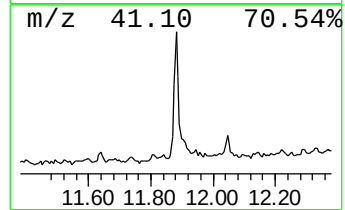
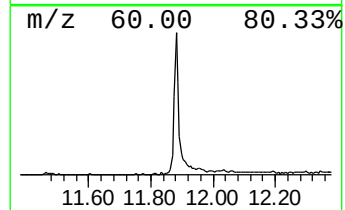
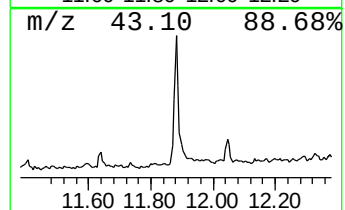
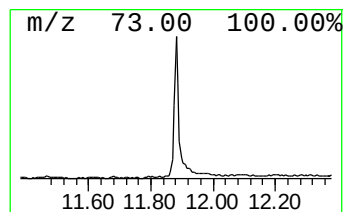
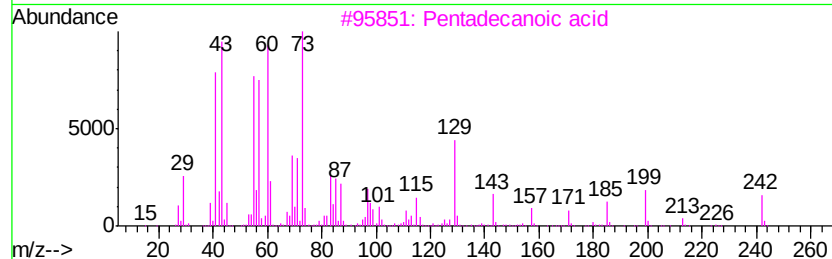
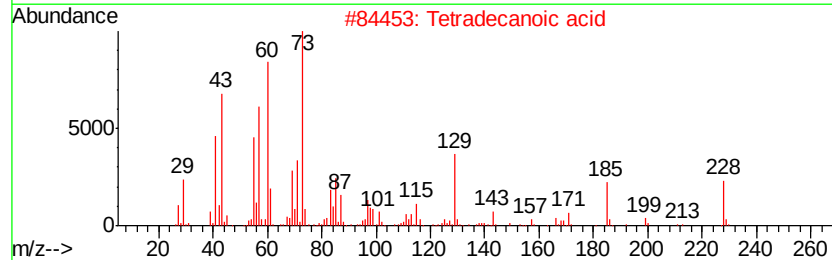
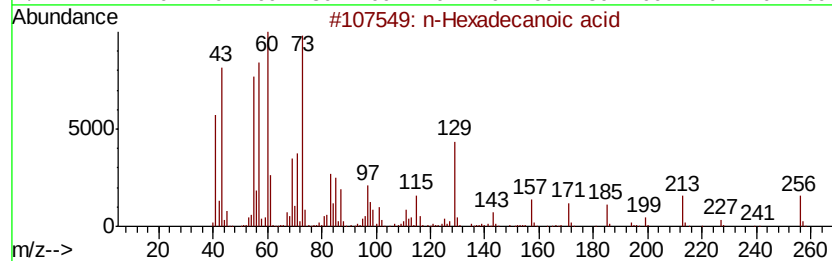
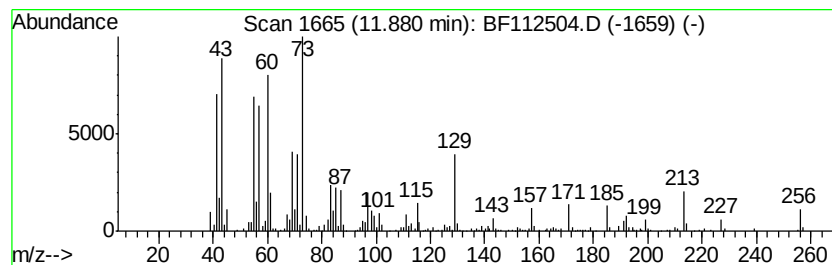
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	13.59 ng	563784	Phenanthrene-d10	11.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4		Tridecanoic acid	214	C13H26O2	000638-53-9	81
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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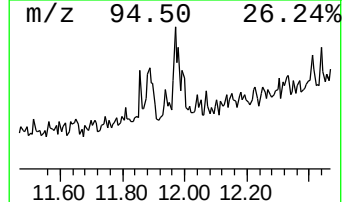
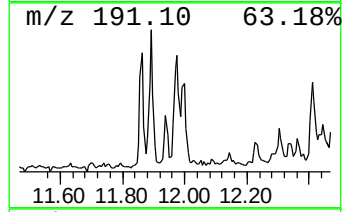
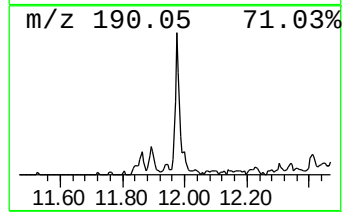
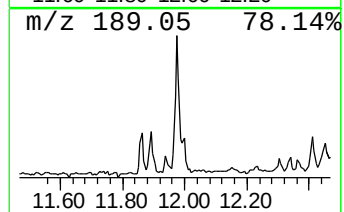
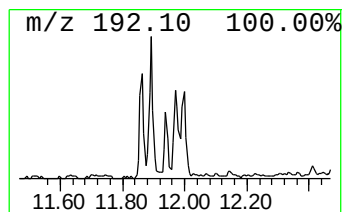
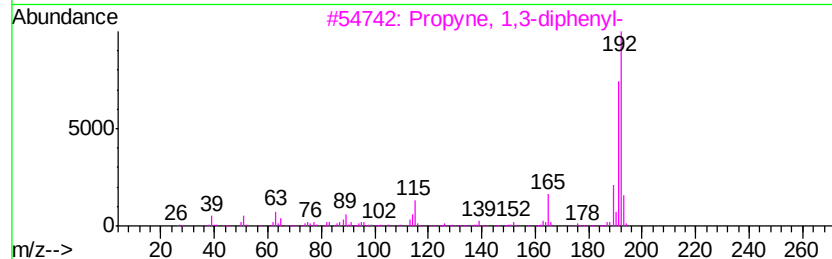
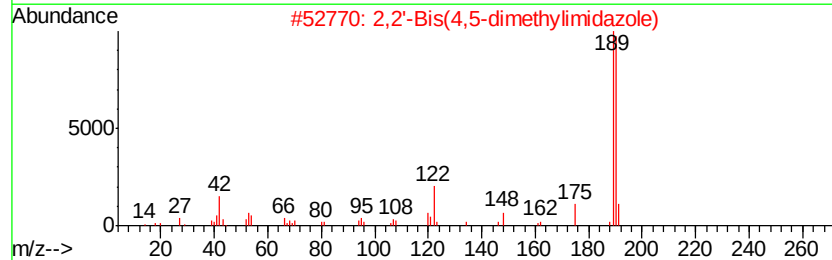
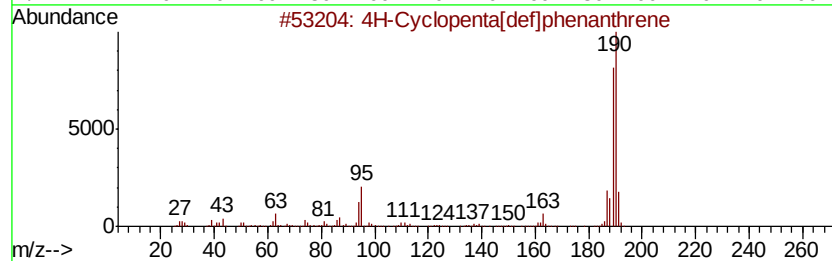
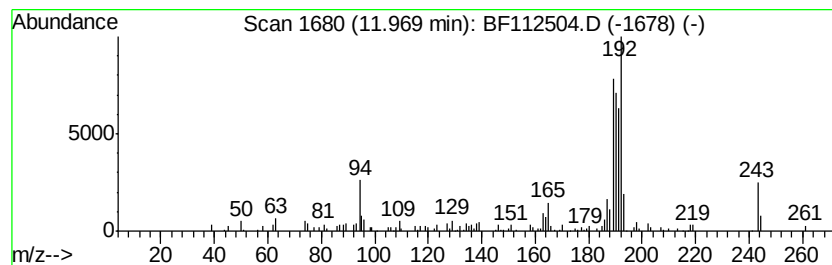
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.97	2.07 ng	85825	Phenanthrene-d10	11.36	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	43
3	Propyne, 1,3-diphenyl-	192	C15H12	004980-70-5	18
4	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	18
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	18



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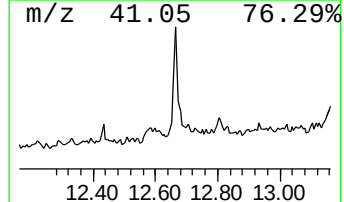
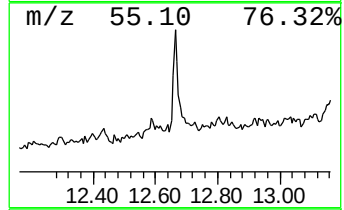
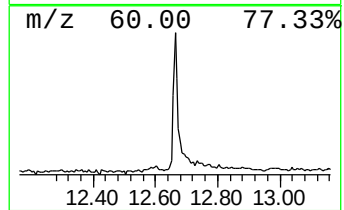
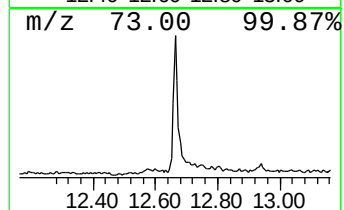
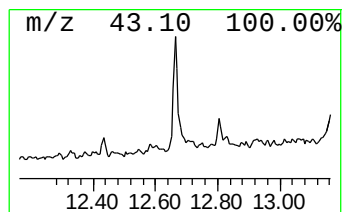
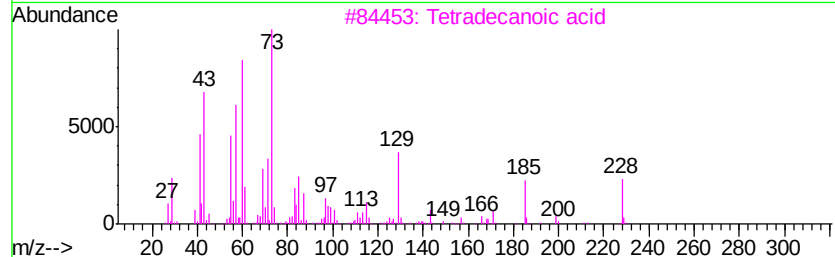
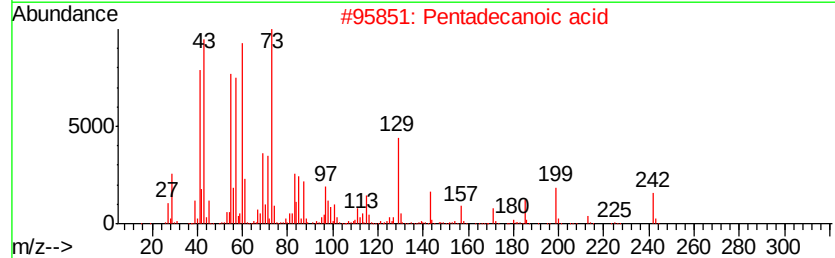
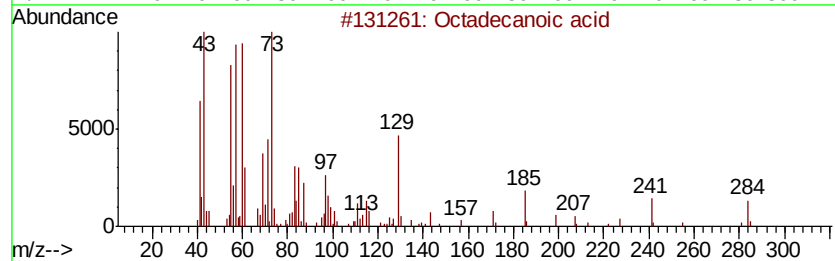
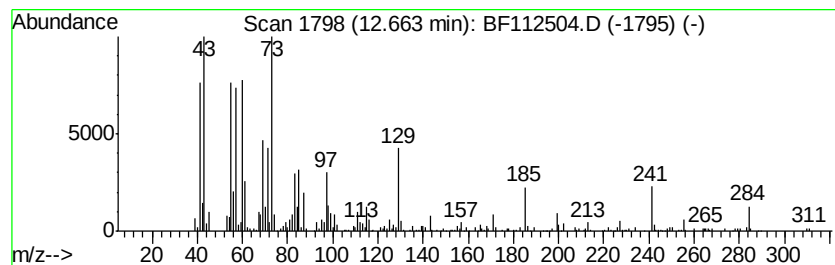
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	8.14 ng	337596	Phenanthrene-d10	11.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Nonadecane	268	C19H40	000629-92-5	56
5		Hexadecane	226	C16H34	000544-76-3	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112504.D
Acq On : 12 Feb 2019 11:26
Operator : JU/SJ
Sample : K1442-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-11

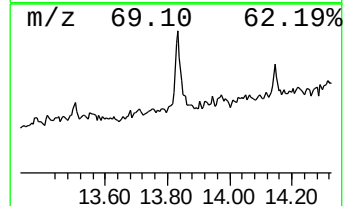
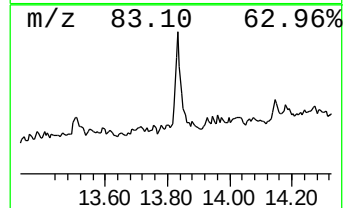
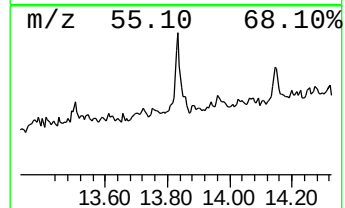
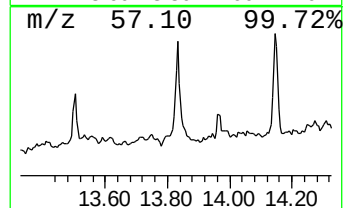
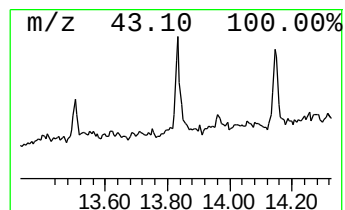
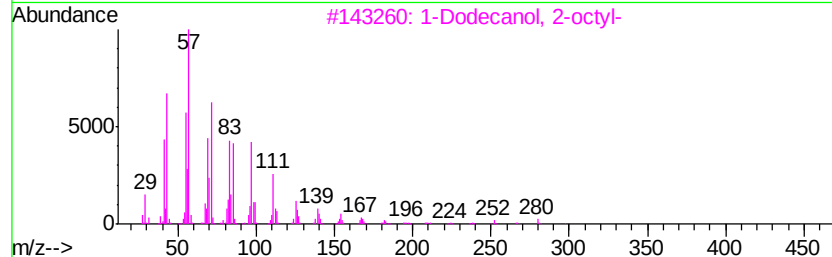
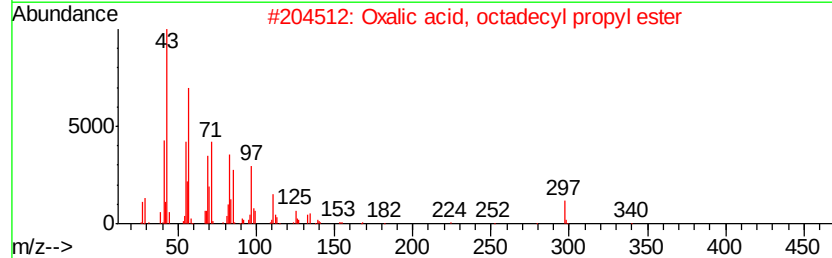
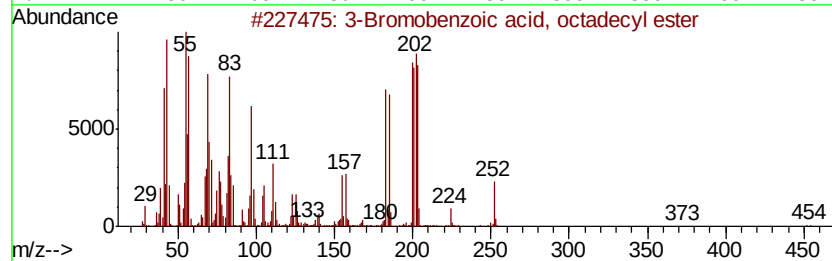
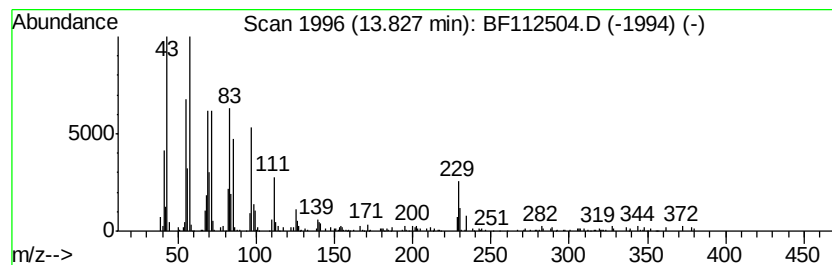
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 3-Bromobenzoic acid, octade... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.62 ng	187440	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Bromobenzoic acid, octadecyl e...	452	C25H41BrO2	070153-14-9	95
2		Oxalic acid, octadecyl propyl ester	384	C23H44O4	1000309-27-0	90
3		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
5		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
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Sample : K1442-05
Misc :
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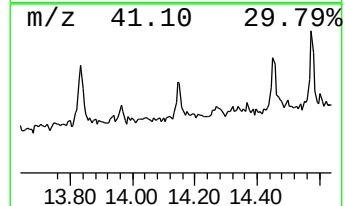
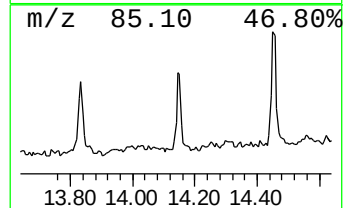
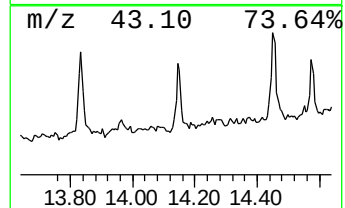
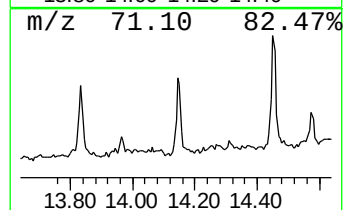
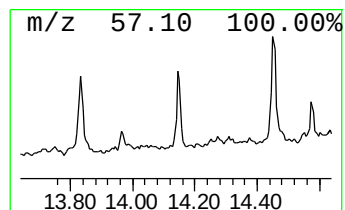
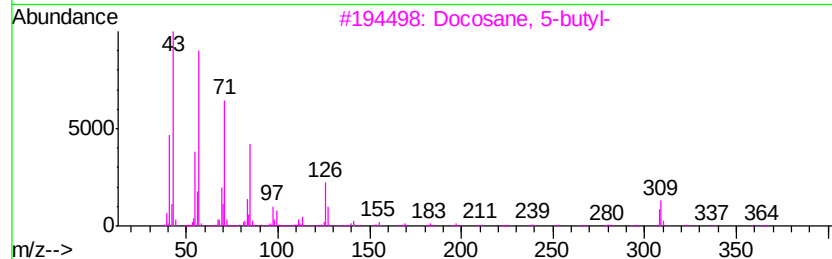
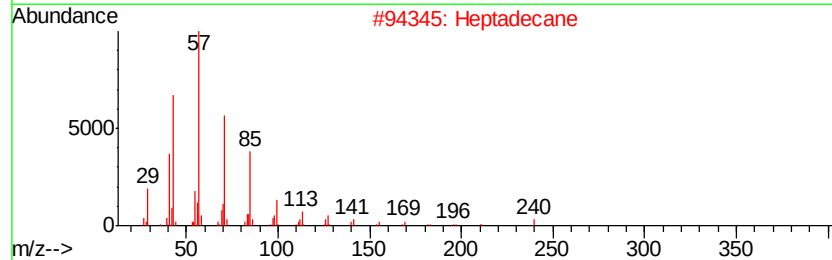
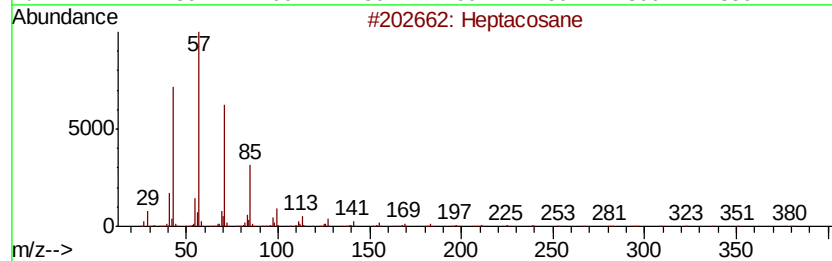
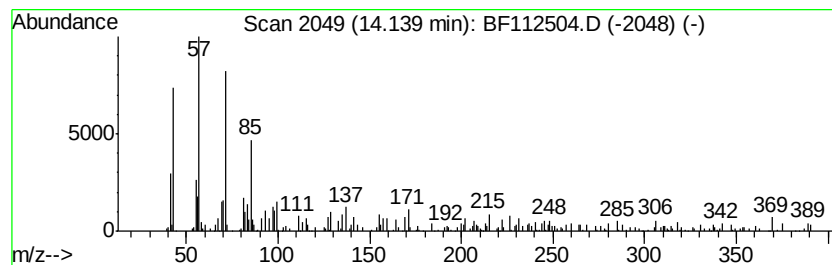
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	3.32 ng	171871	Chrysene-d12	14.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	90
2	Heptadecane		240	C17H36	000629-78-7	89
3	Docosane, 5-butyl-		366	C26H54	055282-16-1	89
4	Hexacosane		366	C26H54	000630-01-3	76
5	Octadecane, 2-methyl-		268	C19H40	001560-88-9	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112504.D
Acq On : 12 Feb 2019 11:26
Operator : JU/SJ
Sample : K1442-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

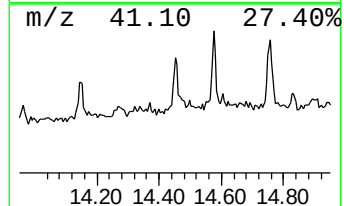
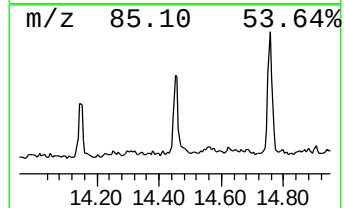
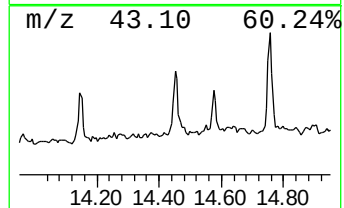
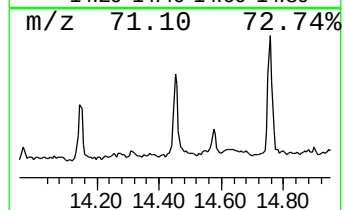
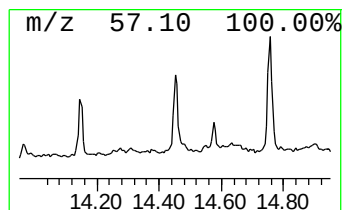
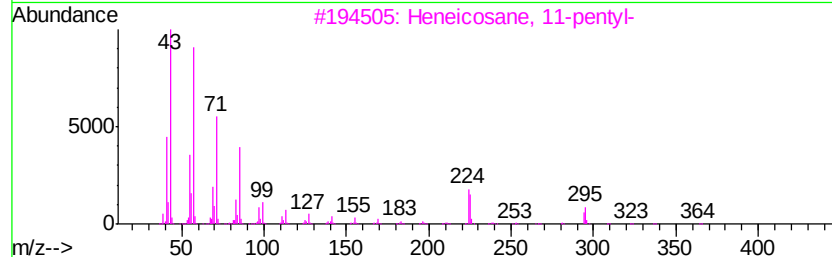
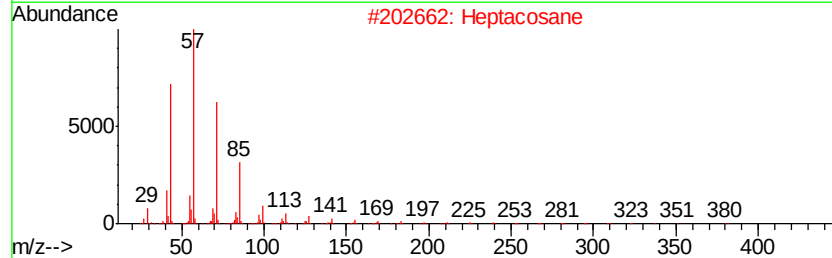
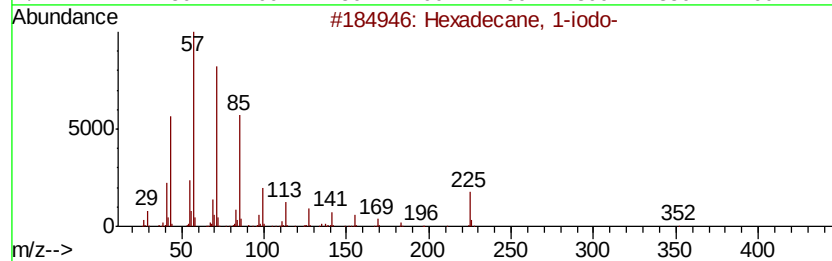
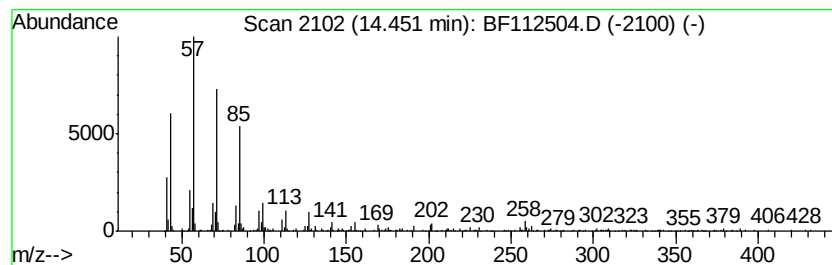
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	4.44 ng	230119	Chrysene-d12	14.01
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane, 1-iodo-	352 C16H33I	000544-77-4	95
2	Heptacosane	380 C27H56	000593-49-7	93
3	Heneicosane, 11-pentyl-	366 C26H54	014739-72-1	93
4	Docosane, 9-butyl-	366 C26H54	055282-14-9	93
5	Eicosane	282 C20H42	000112-95-8	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
Data File : BF112504.D
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Operator : JU/SJ
Sample : K1442-05
Misc :
ALS Vial : 4 Sample Multiplier: 1

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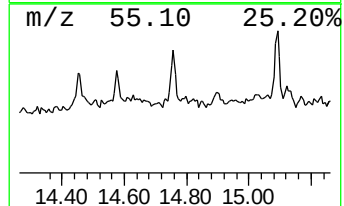
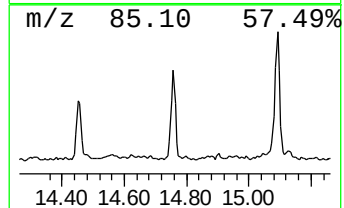
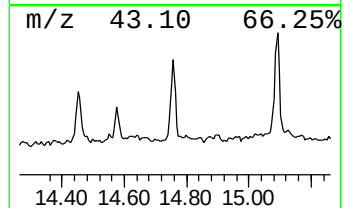
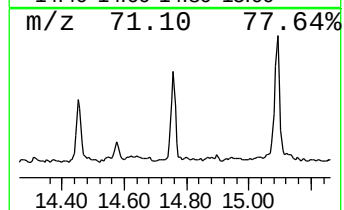
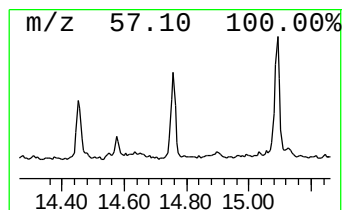
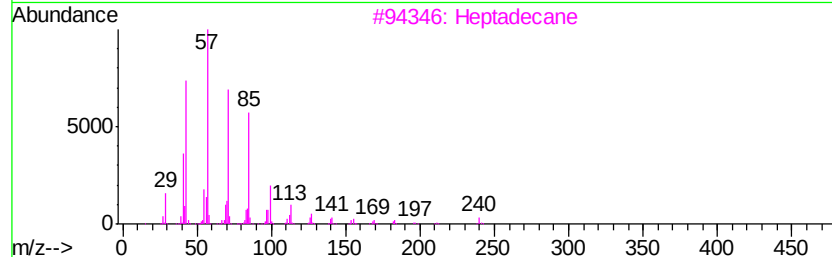
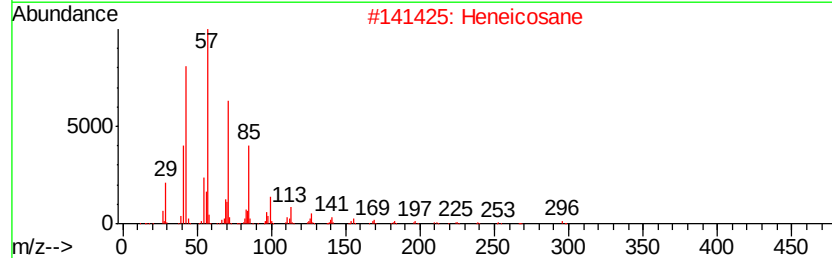
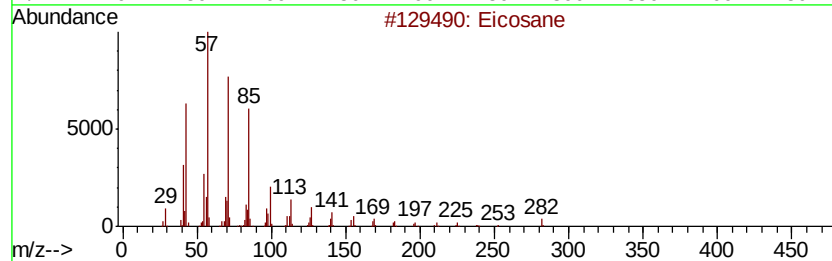
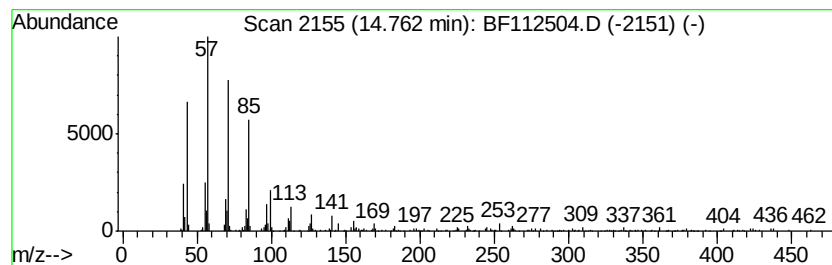
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	6.60 ng	306319	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	95
2		Heneicosane	296	C21H44	000629-94-7	94
3		Heptadecane	240	C17H36	000629-78-7	94
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021219\
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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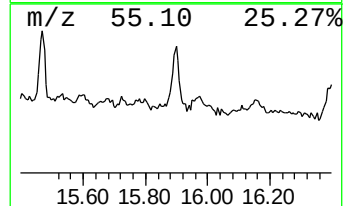
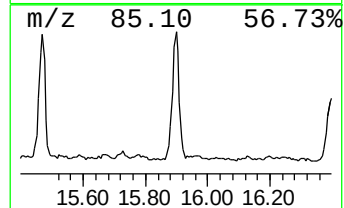
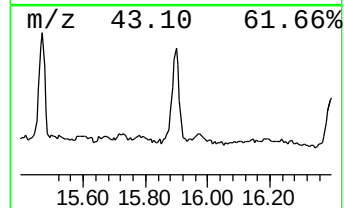
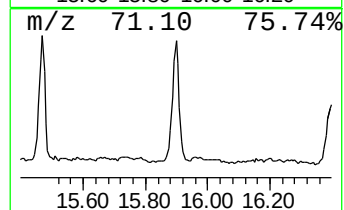
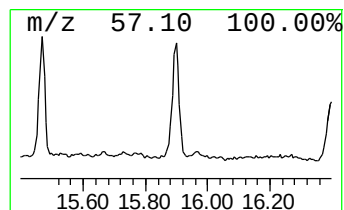
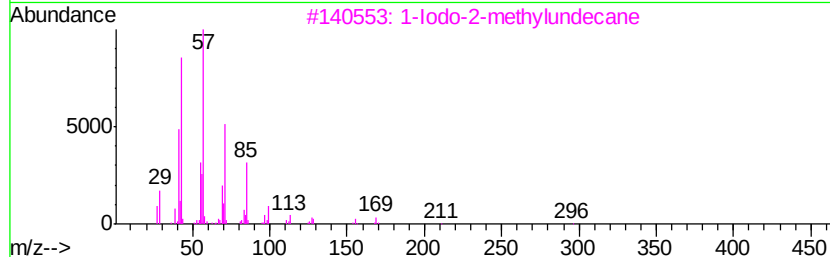
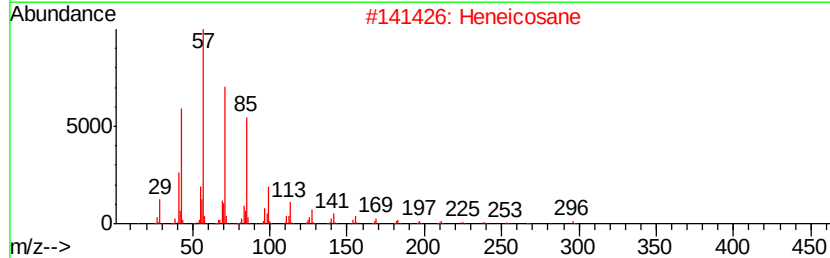
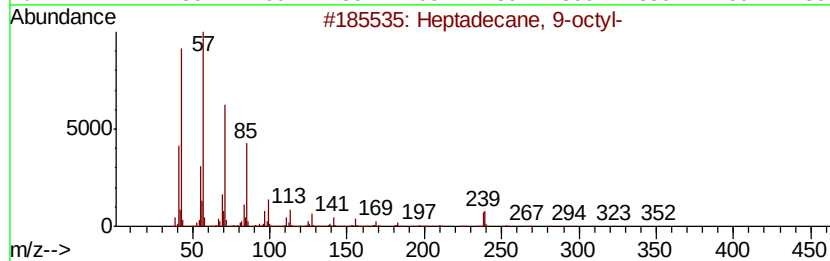
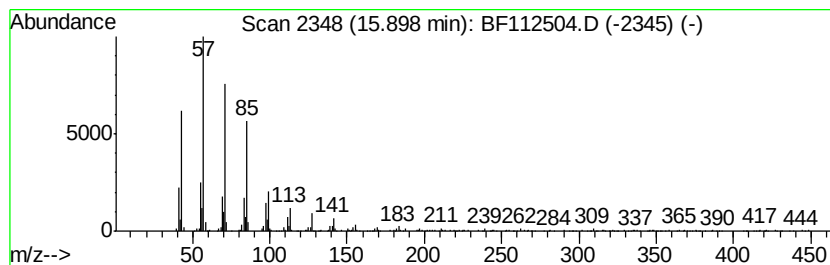
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	12.31 ng	571178	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Tetratetracontane	619	C44H90	007098-22-8	90



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Misc :
ALS Vial : 4 Sample Multiplier: 1

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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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unknown6.61	6.61	76.9	ng	2876990	1	6.83	748070	20.0
n-Hexadecanoic acid	11.88	13.6	ng	563784	4	11.36	829539	20.0
4H-Cyclopenta[def...	11.97	2.1	ng	85825	4	11.36	829539	20.0
Octadecanoic acid	12.66	8.1	ng	337596	4	11.36	829539	20.0
3-Bromobenzoic ac...	13.83	3.6	ng	187440	5	14.01	1036500	20.0
Heptacosane	14.14	3.3	ng	171871	5	14.01	1036500	20.0
Hexadecane, 1-iodo-	14.45	4.4	ng	230119	5	14.01	1036500	20.0
Eicosane	14.76	6.6	ng	306319	6	15.49	928246	20.0
Heptadecane, 9-oc...	15.90	12.3	ng	571178	6	15.49	928246	20.0