

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
 Data File : BF110209.D
 Acq On : 26 Oct 2018 15:02
 Operator : JU/SJ
 Sample : J5621-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SA-SED-02

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-BF102318.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.310	33	38	47	rVB	354935	461527	14.10%	1.672%
2	5.210	527	531	539	rBV	105061	132149	4.04%	0.479%
3	5.592	591	596	599	rBV	2818409	2740500	83.71%	9.927%
4	6.592	760	766	776	rBV2	2638360	3273921	100.00%	11.859%
5	6.739	786	791	794	rBV	3170934	2912826	88.97%	10.551%
6	6.969	826	830	833	rBV	1008248	840151	25.66%	3.043%
7	7.122	852	856	860	rBV	2355914	2162368	66.05%	7.833%
8	7.533	920	926	929	rBV	1756156	1811626	55.34%	6.562%
9	8.251	1044	1048	1051	rBV	1252064	1057111	32.29%	3.829%
10	9.327	1225	1231	1234	rBV	3122752	3003690	91.75%	10.880%
11	9.716	1293	1297	1304	rVB	366191	299473	9.15%	1.085%
12	10.010	1343	1347	1351	rBV2	1231524	1089803	33.29%	3.948%
13	10.804	1477	1482	1495	rBV	1566865	1490813	45.54%	5.400%
14	11.504	1597	1601	1604	rBV	1119709	930067	28.41%	3.369%
15	12.010	1683	1687	1690	rBV	86840	86515	2.64%	0.313%
16	12.721	1804	1808	1813	rBV	95409	97254	2.97%	0.352%
17	12.892	1834	1837	1840	rVB	90362	72189	2.20%	0.261%
18	12.951	1841	1847	1852	rVB	109626	145444	4.44%	0.527%
19	13.086	1866	1870	1873	rBV	2384644	1987462	60.71%	7.199%
20	13.598	1954	1957	1960	rBV	68253	56310	1.72%	0.204%
21	13.639	1962	1964	1967	rVB2	46990	42298	1.29%	0.153%
22	13.974	2018	2021	2024	rBV	84964	97354	2.97%	0.353%
23	14.151	2047	2051	2054	rBV	817282	754510	23.05%	2.733%
24	14.286	2072	2074	2077	rVB	89044	71446	2.18%	0.259%
25	14.592	2123	2126	2134	rVB	154551	162936	4.98%	0.590%
26	14.915	2177	2181	2185	rBV	202152	216847	6.62%	0.785%
27	15.268	2238	2241	2245	rVB	269503	311011	9.50%	1.127%
28	15.674	2305	2310	2316	rBV2	558227	816715	24.95%	2.958%
29	16.133	2384	2388	2395	rVB	184584	300987	9.19%	1.090%
30	16.674	2476	2480	2486	rVB	99203	181276	5.54%	0.657%

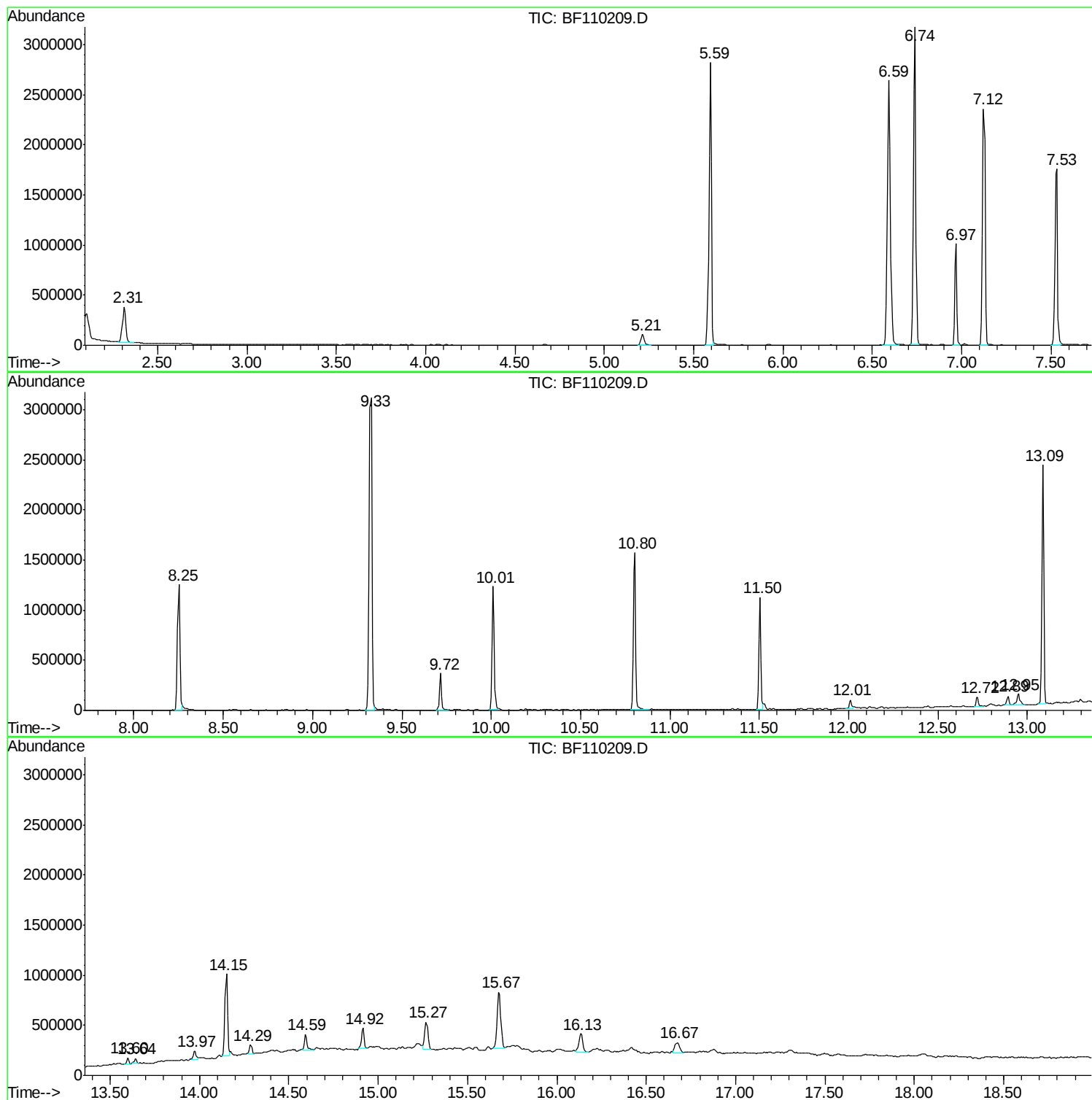
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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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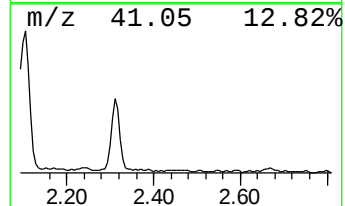
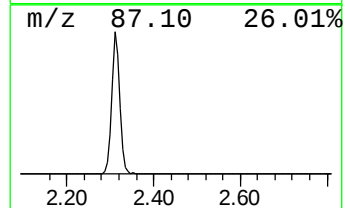
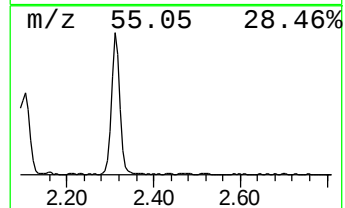
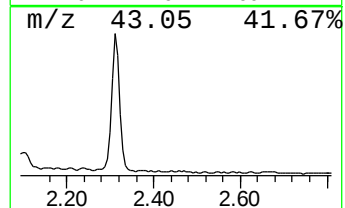
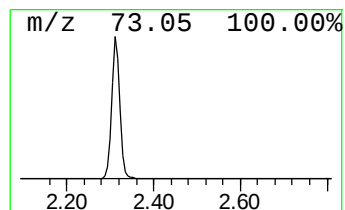
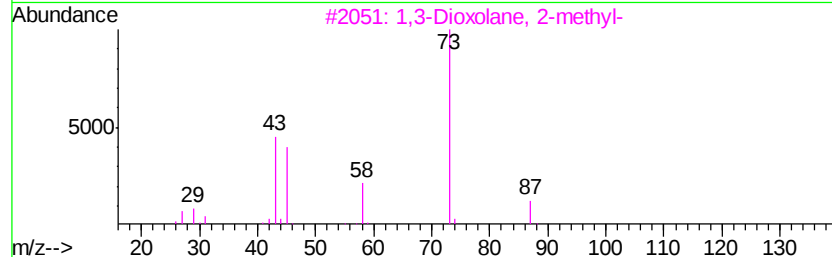
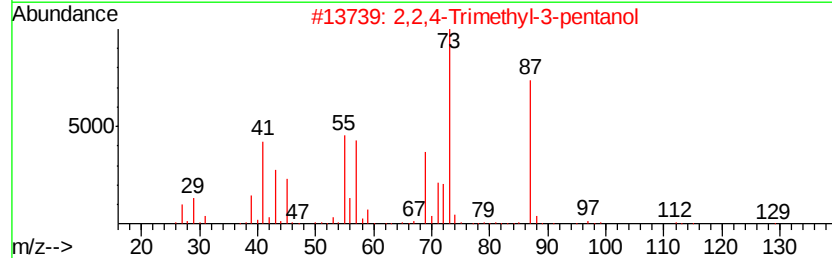
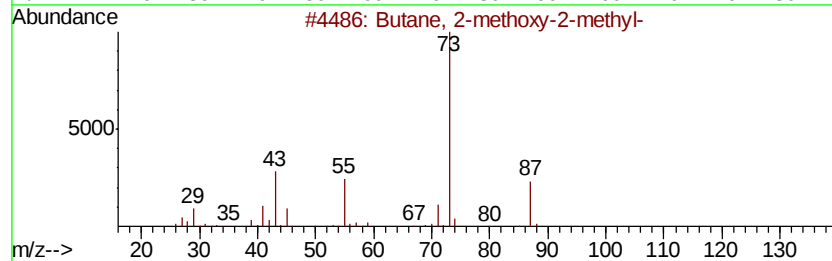
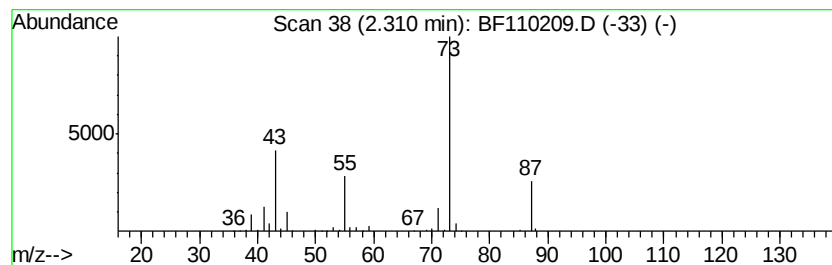
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	10.99 ng	461527	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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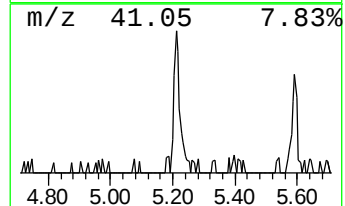
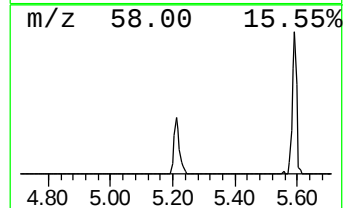
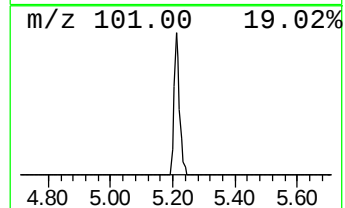
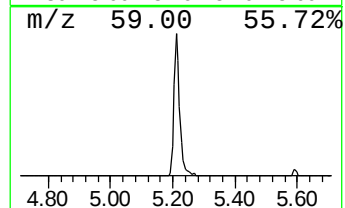
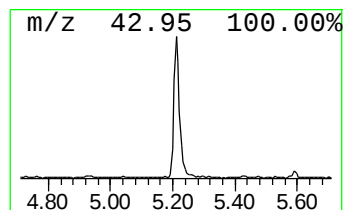
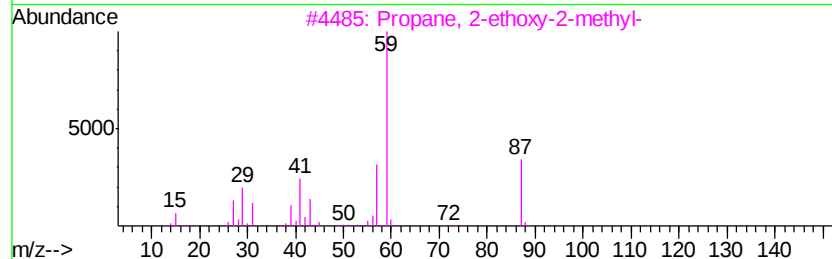
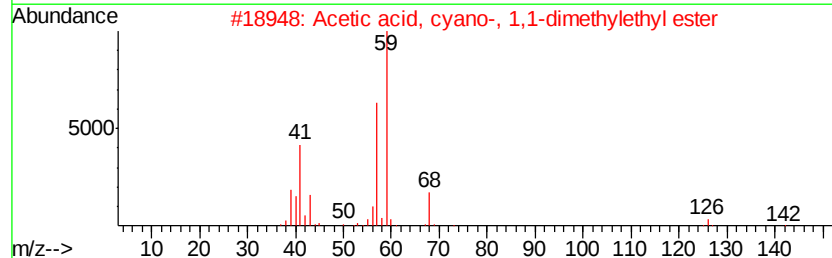
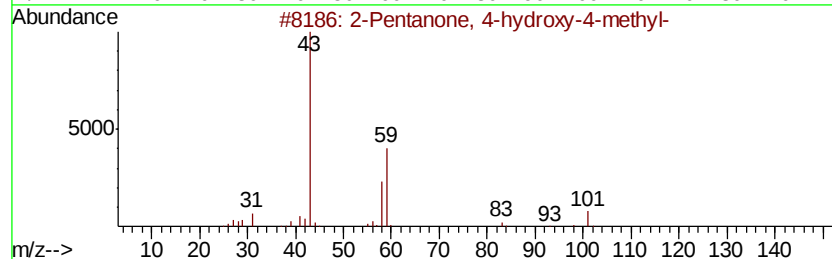
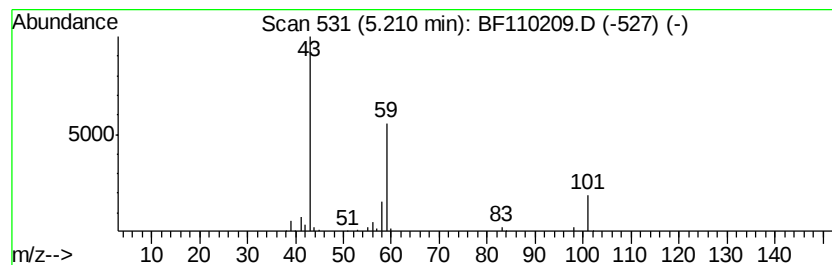
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	3.15 ng	132149	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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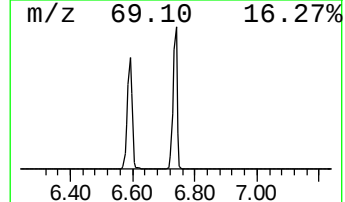
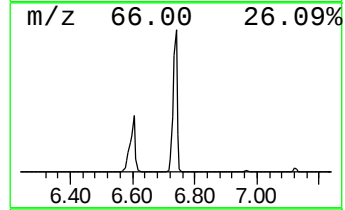
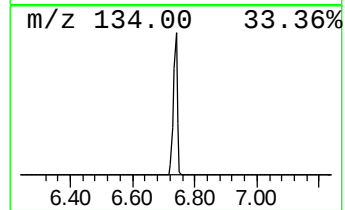
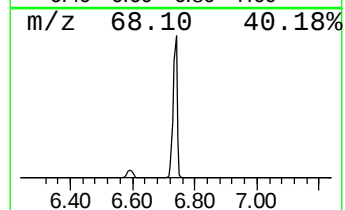
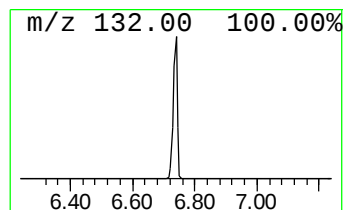
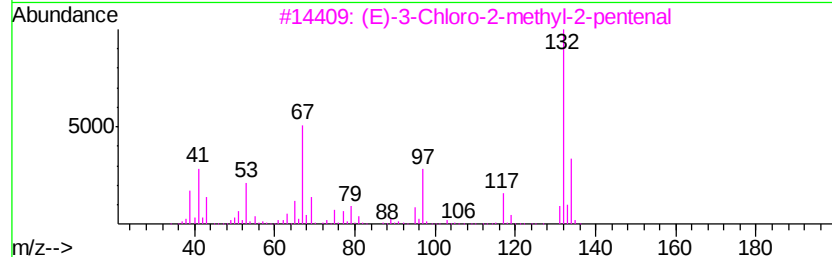
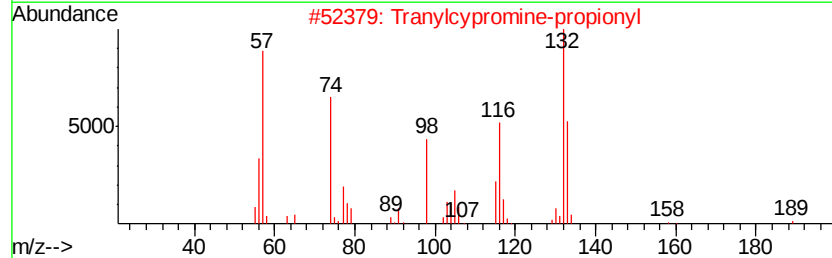
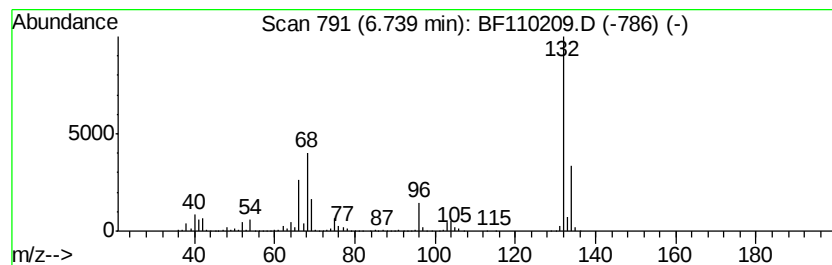
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Peak Number 3 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	69.34 ng	2912830	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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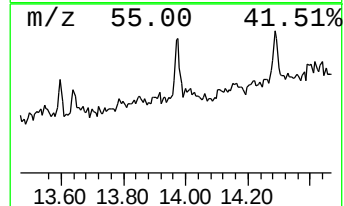
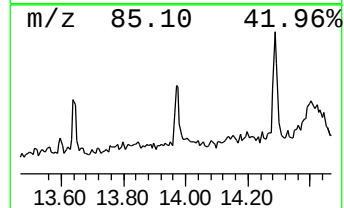
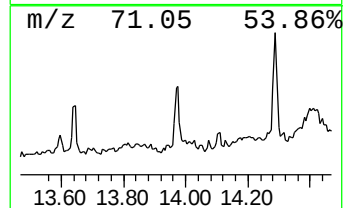
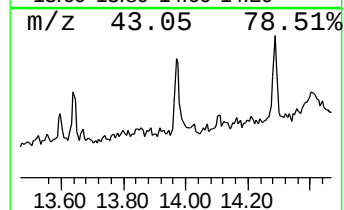
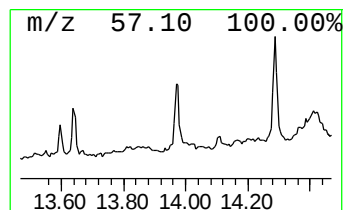
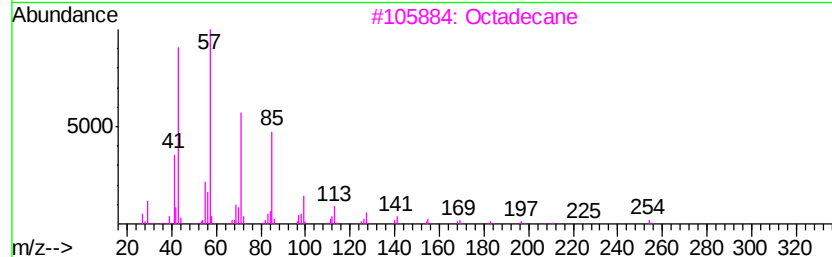
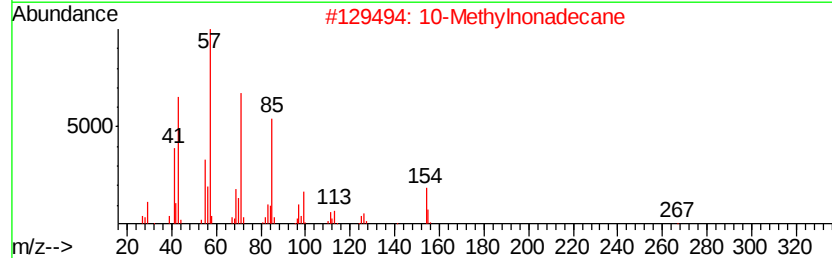
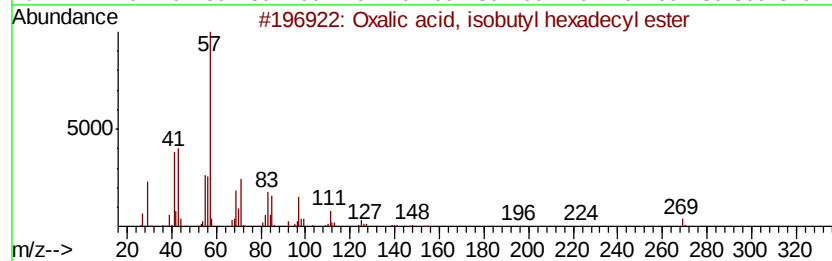
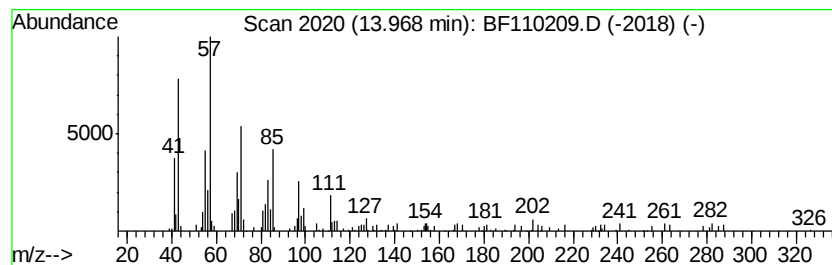
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Peak Number 6 Oxalic acid, isobutyl hexad... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.58 ng	97354	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	64
2		10-Methylnonadecane	282	C20H42	056862-62-5	62
3		Octadecane	254	C18H38	000593-45-3	60
4		Pentadecane	212	C15H32	000629-62-9	53
5		Nonadecane	268	C19H40	000629-92-5	52



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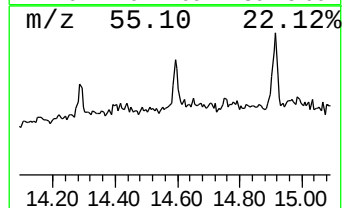
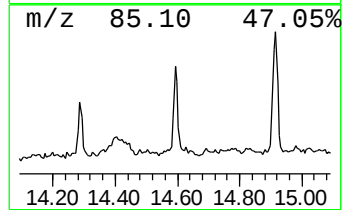
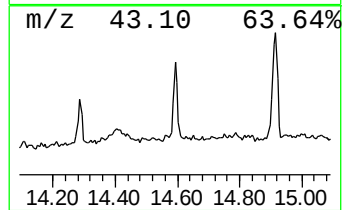
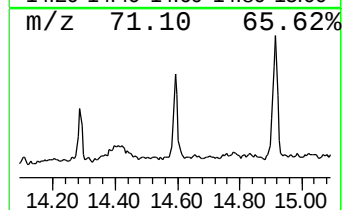
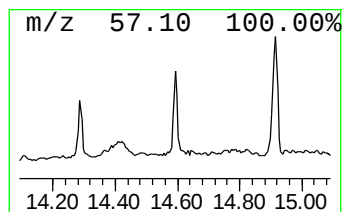
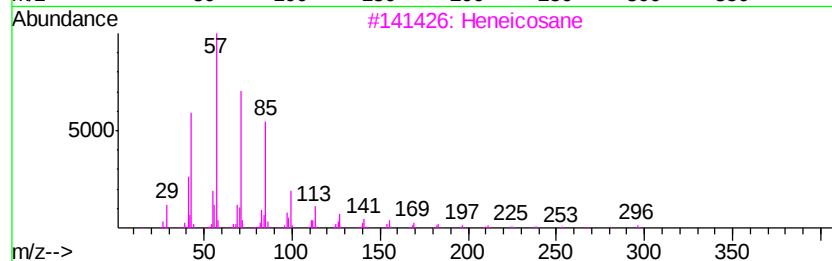
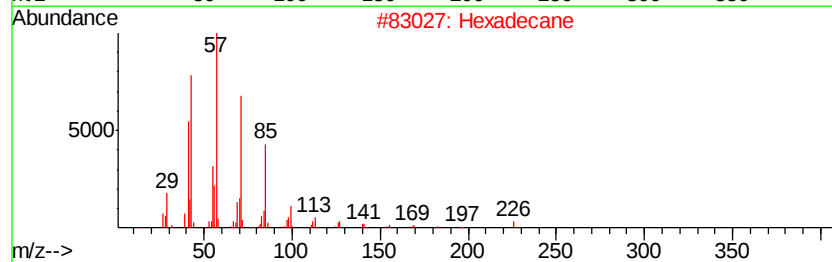
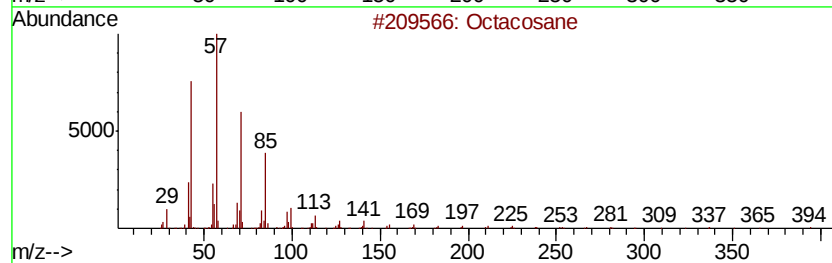
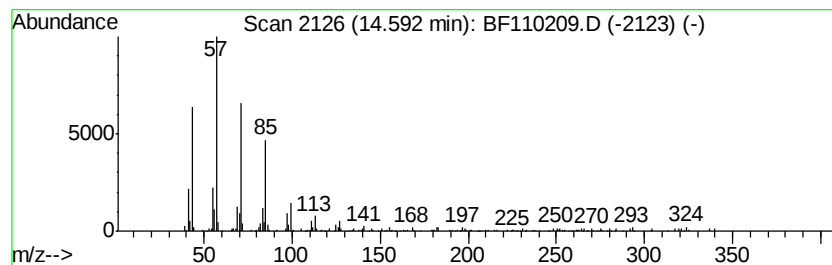
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	4.32 ng	162936	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	Heneicosane		296	C21H44	000629-94-7	87
4	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	80
5	Heptacosane		380	C27H56	000593-49-7	68



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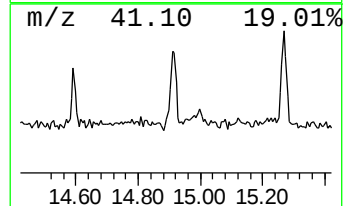
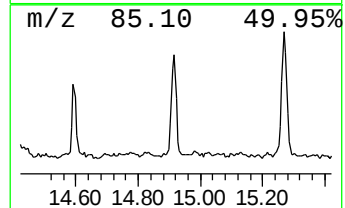
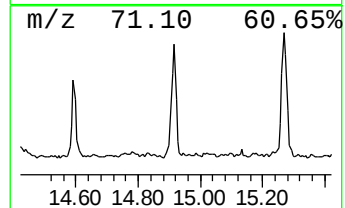
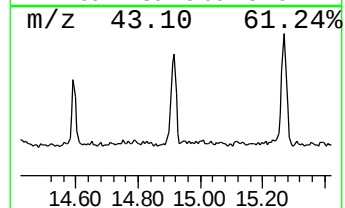
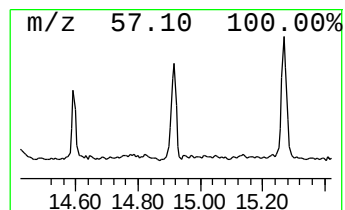
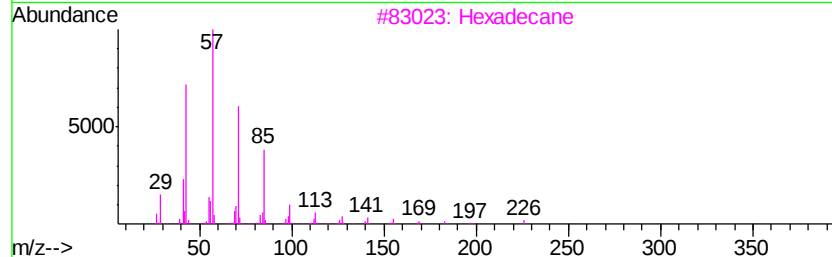
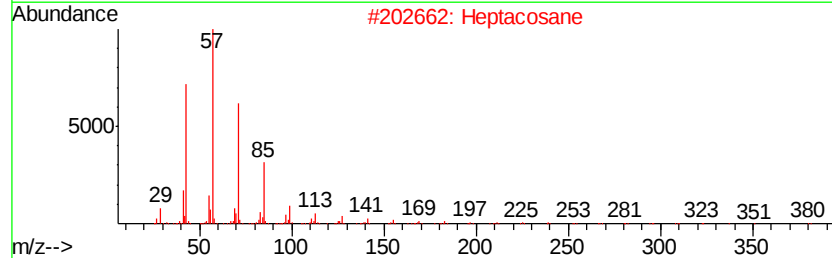
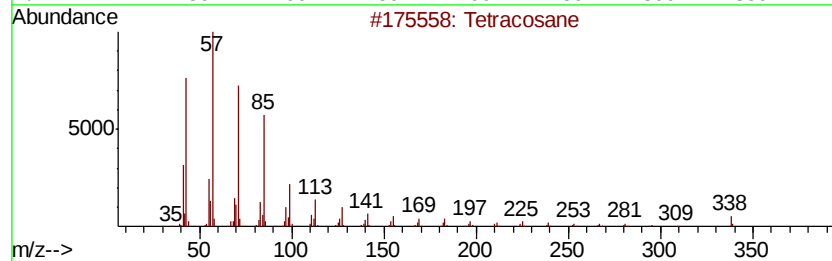
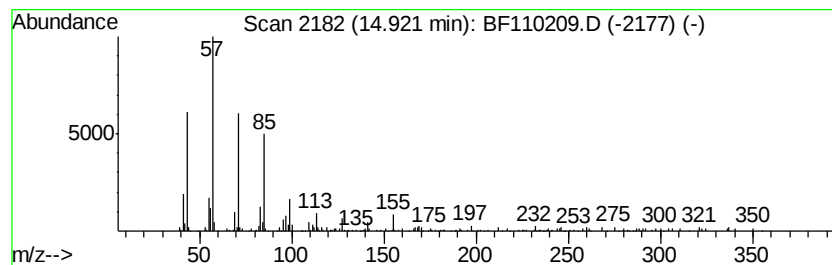
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	5.75 ng	216847	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	94
2		Heptacosane	380	C27H56	000593-49-7	91
3		Hexadecane	226	C16H34	000544-76-3	91
4		Nonadecane	268	C19H40	000629-92-5	90
5		Pentadecane	212	C15H32	000629-62-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
Data File : BF110209.D
Acq On : 26 Oct 2018 15:02
Operator : JU/SJ
Sample : J5621-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-SED-02

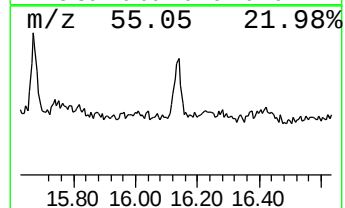
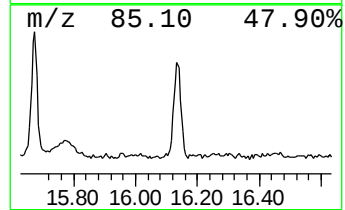
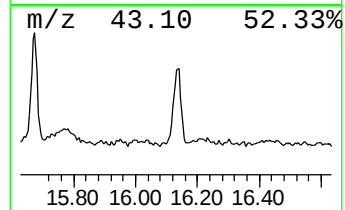
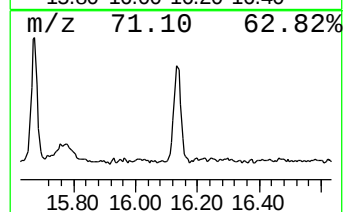
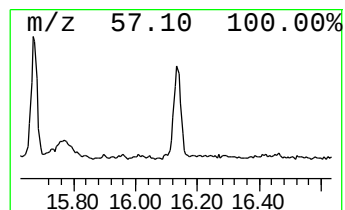
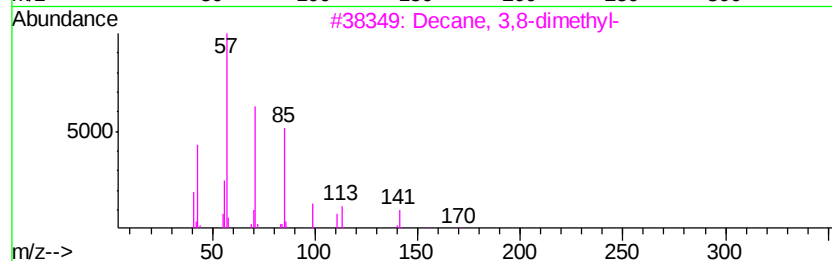
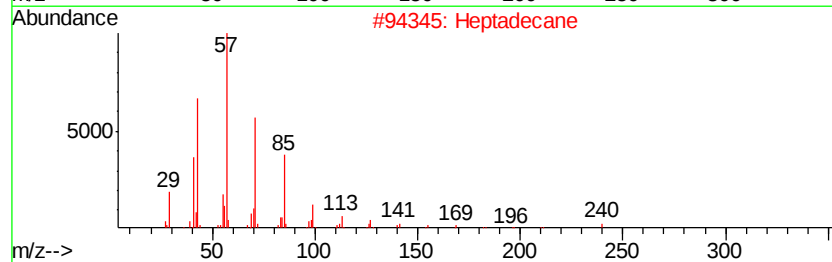
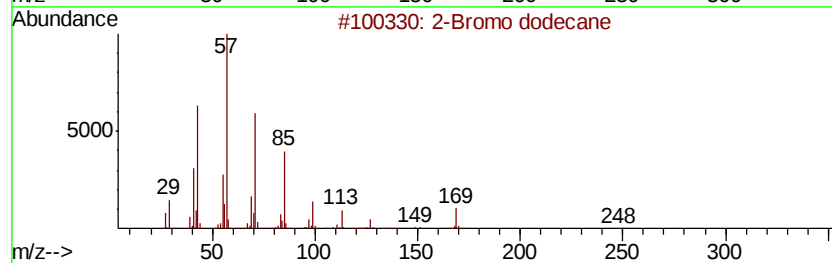
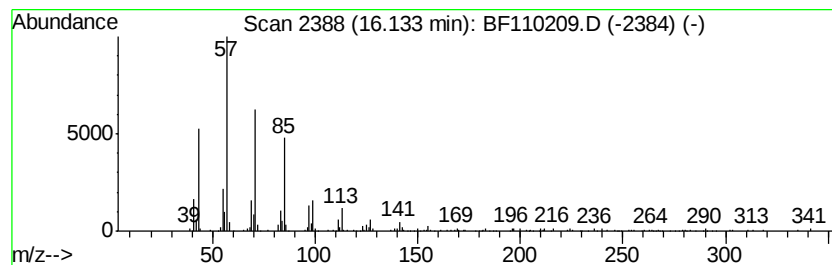
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Bromo dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	7.37 ng	300987	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2		Heptadecane	240	C17H36	000629-78-7	90
3		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
4		Octacosane	394	C28H58	000630-02-4	86
5		Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102618\
Data File : BF110209.D
Acq On : 26 Oct 2018 15:02
Operator : JU/SJ
Sample : J5621-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-SED-02

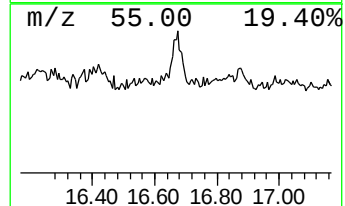
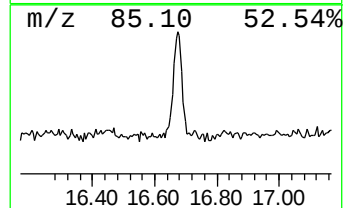
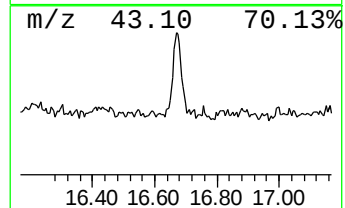
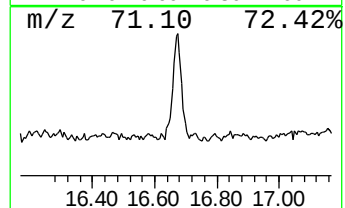
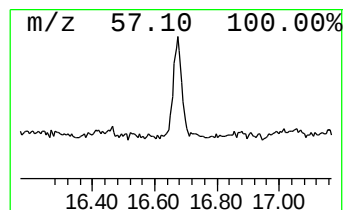
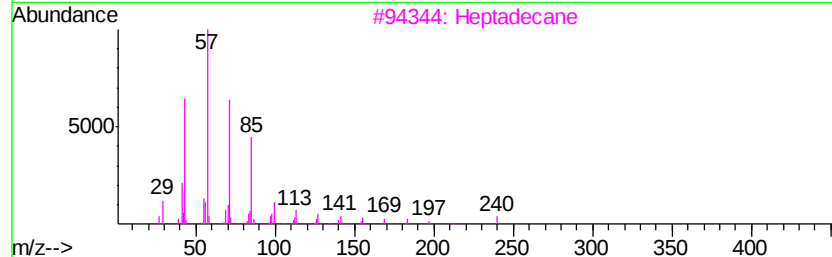
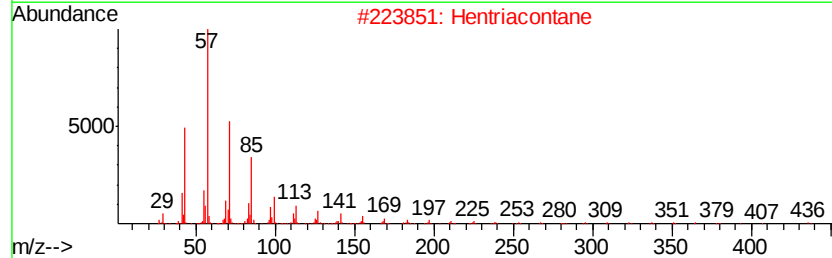
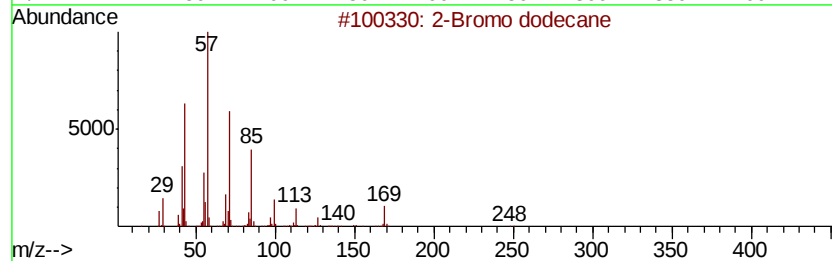
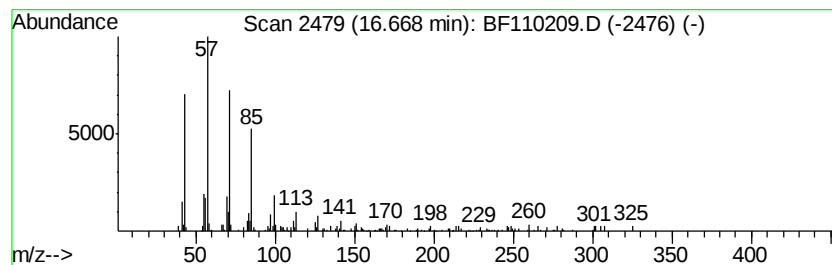
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.67	4.44 ng	181276	Perylene-d12	15.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
2		Hentriacontane	437	C31H64	000630-04-6	86
3		Heptadecane	240	C17H36	000629-78-7	86
4		Pentadecane	212	C15H32	000629-62-9	86
5		Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102618\
Data File : BF110209.D
Acq On : 26 Oct 2018 15:02
Operator : JU/SJ
Sample : J5621-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SA-SED-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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
Butane, 2-methoxy...	2.31	11.0	ng	461527	1	6.97	840151	20.0
2-Pentanone, 4-hy...	5.21	3.1	ng	132149	1	6.97	840151	20.0
unknown6.74	6.74	69.3	ng	2912830	1	6.97	840151	20.0
Oxalic acid, isob...	13.97	2.6	ng	97354	5	14.15	754510	20.0
Octacosane	14.59	4.3	ng	162936	5	14.15	754510	20.0
Tetracosane	14.92	5.8	ng	216847	5	14.15	754510	20.0
2-Bromo dodecane	16.13	7.4	ng	300987	6	15.68	816715	20.0
Hentriacontane	16.67	4.4	ng	181276	6	15.68	816715	20.0