

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121518\
 Data File : BF111461.D
 Acq On : 15 Dec 2018 11:50
 Operator : JU/SJ
 Sample : J6208-09
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3

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-BF121418.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	4.999	492	495	502	rVB	138988	169121	4.66%	0.451%
2	5.422	562	567	570	rBV	3468262	3163439	87.10%	8.443%
3	6.440	735	740	753	rBV	3520787	3632001	100.00%	9.694%
4	6.569	757	762	765	rBV	3840608	3361249	92.55%	8.971%
5	6.793	796	800	809	rBV	1330579	1058825	29.15%	2.826%
6	6.951	823	827	830	rBV	3104181	2512991	69.19%	6.707%
7	7.351	890	895	898	rBV	2305458	2125807	58.53%	5.674%
8	8.075	1014	1018	1034	rBV	1665280	1418665	39.06%	3.786%
9	9.151	1197	1201	1204	rBV	3853703	3192832	87.91%	8.522%
10	9.545	1264	1268	1275	rBV	202203	201766	5.56%	0.539%
11	9.828	1312	1316	1320	rBV	1603485	1464362	40.32%	3.908%
12	10.616	1446	1450	1463	rBV	1848838	1685410	46.40%	4.498%
13	11.310	1565	1568	1571	rBV	1304115	1305685	35.95%	3.485%
14	11.333	1571	1572	1576	rVV	457470	326296	8.98%	0.871%
15	11.386	1576	1581	1585	rVB	102332	111500	3.07%	0.298%
16	11.545	1603	1608	1610	rBV2	42282	55765	1.54%	0.149%
17	11.816	1651	1654	1655	rBV	88868	82333	2.27%	0.220%
18	11.851	1655	1660	1669	rVB2	1369514	1722446	47.42%	4.597%
19	11.928	1669	1673	1675	rBV2	97791	104218	2.87%	0.278%
20	12.110	1701	1704	1706	rBV	64252	66827	1.84%	0.178%
21	12.133	1706	1708	1712	rVB2	45664	43519	1.20%	0.116%
22	12.263	1724	1730	1732	rBV4	37251	59651	1.64%	0.159%
23	12.363	1744	1747	1750	rBV	73674	73749	2.03%	0.197%
24	12.404	1750	1754	1759	rVV6	42312	65452	1.80%	0.175%
25	12.445	1759	1761	1767	rVB4	40791	52492	1.45%	0.140%
26	12.522	1771	1774	1777	rVV	610815	564333	15.54%	1.506%
27	12.551	1777	1779	1788	rVV5	100109	232319	6.40%	0.620%
28	12.633	1788	1793	1805	rVV	1003706	1381972	38.05%	3.688%
29	12.751	1808	1813	1816	rVV	540588	626916	17.26%	1.673%
30	12.804	1819	1822	1828	rVB3	46084	73535	2.02%	0.196%
31	12.898	1834	1838	1841	rBV	2468546	2063903	56.83%	5.508%
32	13.080	1867	1869	1872	rVB2	77869	68198	1.88%	0.182%
33	13.186	1883	1887	1889	rBV2	80819	92403	2.54%	0.247%
34	13.586	1952	1955	1960	rVB	60641	71284	1.96%	0.190%

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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	13.751	1981	1983	1987	rBV3	38896	56815	1.56%	0.152%
36	13.804	1988	1992	2000	rVV2	301355	414308	11.41%	1.106%
37	13.951	2012	2017	2019	rBV2	1190137	1319407	36.33%	3.521%
38	13.974	2019	2021	2027	rVB	281934	259504	7.14%	0.693%
39	14.057	2032	2035	2037	rBV3	45245	45194	1.24%	0.121%
40	14.804	2159	2162	2167	rVB4	76721	91724	2.53%	0.245%
41	14.974	2187	2191	2200	rVB	260912	482898	13.30%	1.289%
42	15.268	2238	2241	2247	rVB	148402	187602	5.17%	0.501%
43	15.327	2247	2251	2257	rBV	187288	247945	6.83%	0.662%
44	15.392	2257	2262	2266	rBV	799223	1014965	27.95%	2.709%
45	16.804	2498	2502	2507	rVB2	67945	116269	3.20%	0.310%

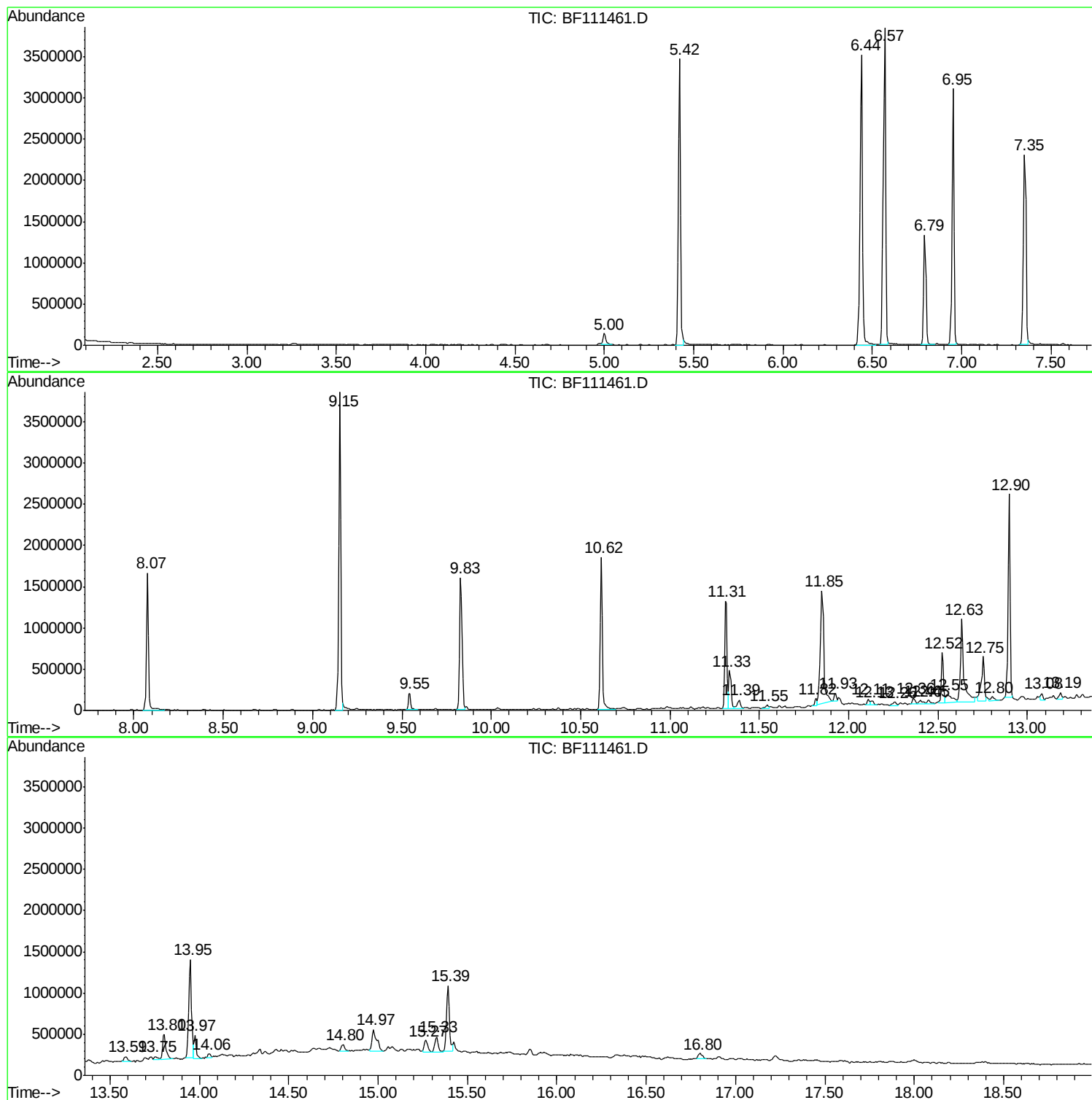
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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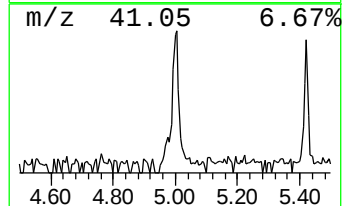
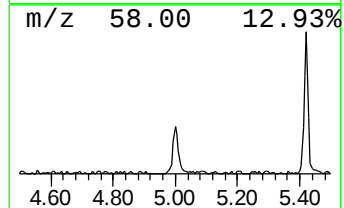
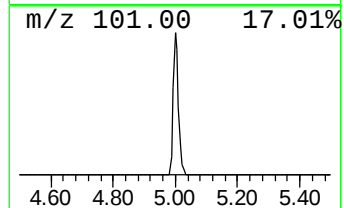
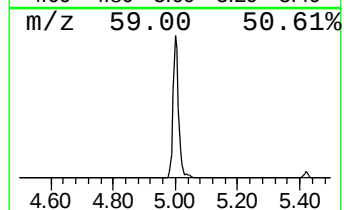
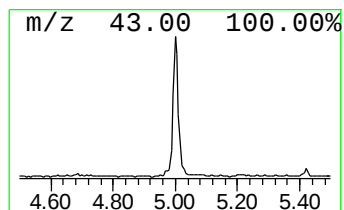
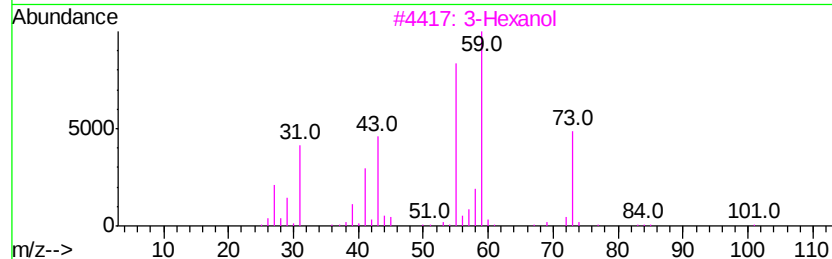
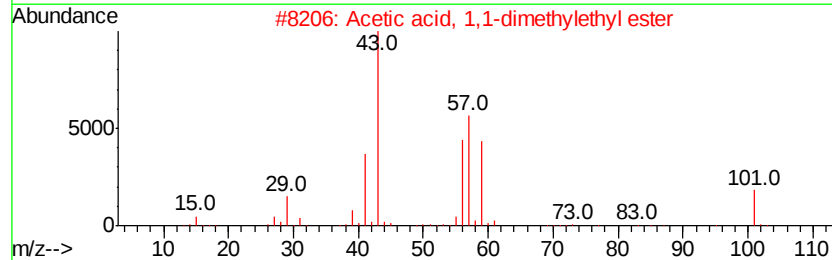
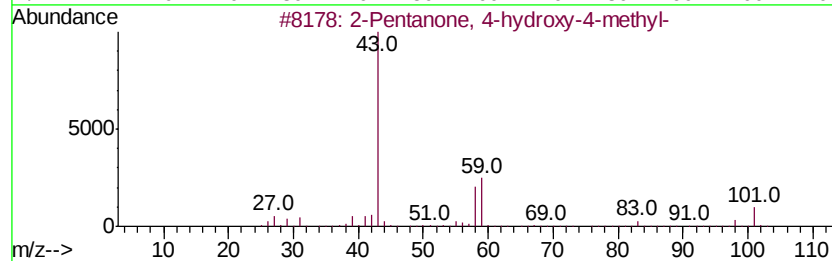
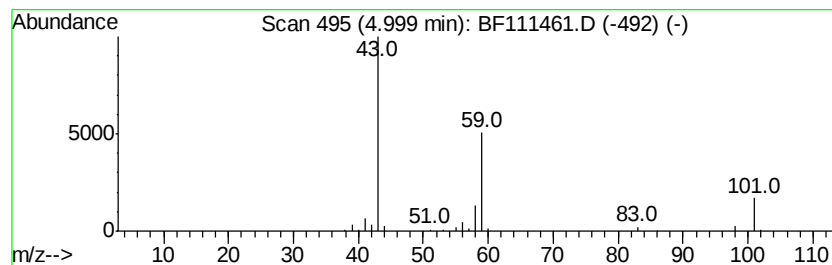
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.19 ng	169121	1,4-Dichlorobenzene-d4	6.79

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	38
3			3-Hexanol	102	C6H14O	000623-37-0	33
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9



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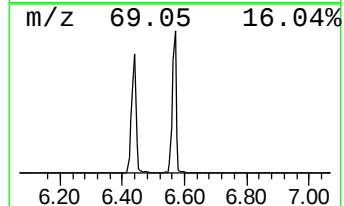
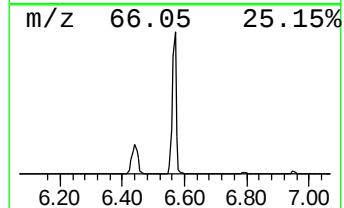
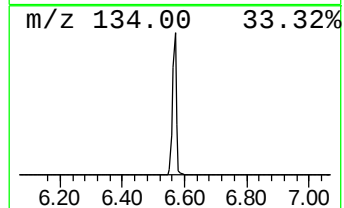
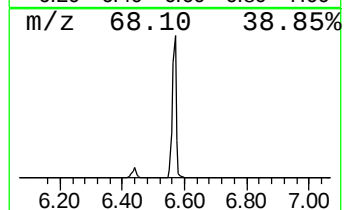
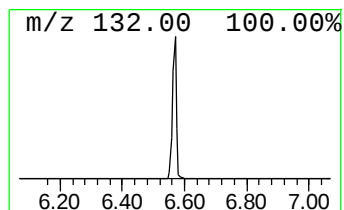
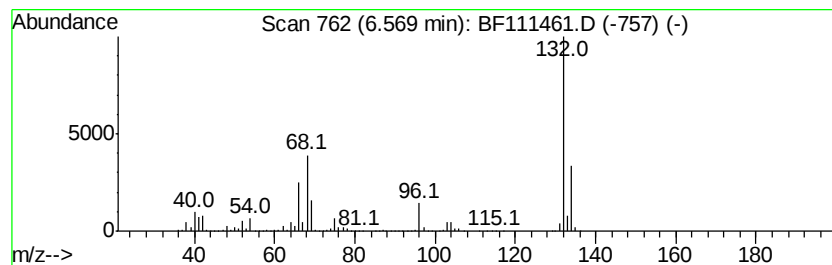
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF121418.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	63.49 ng	3361250	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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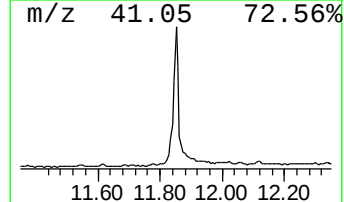
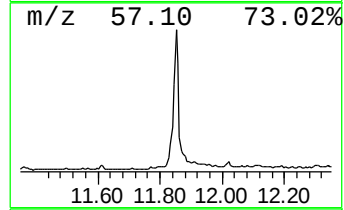
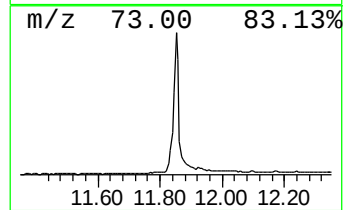
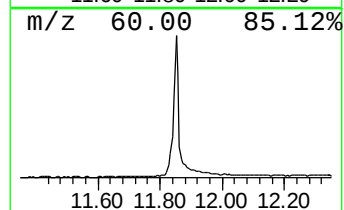
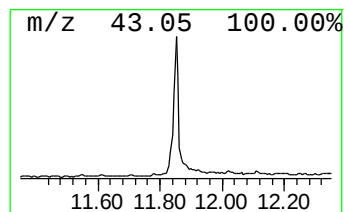
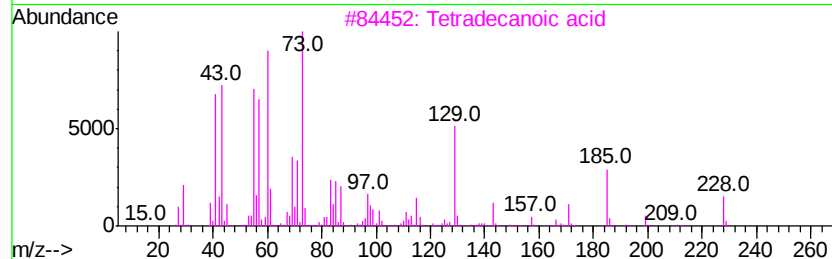
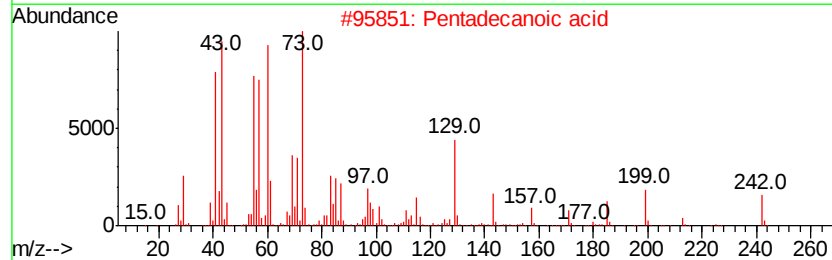
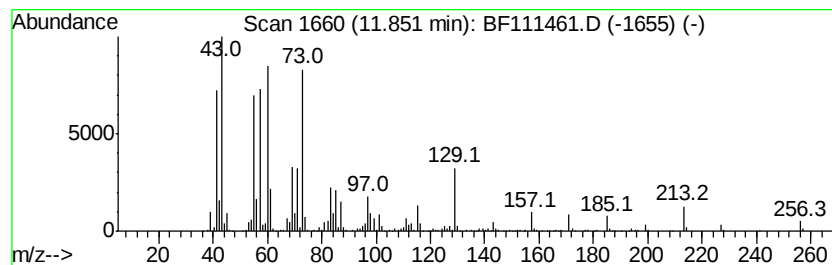
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	26.38 ng	1722450	Phenanthrene-d10	11.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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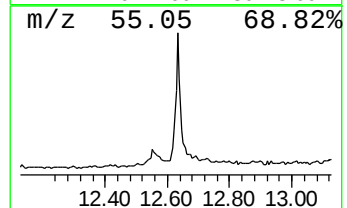
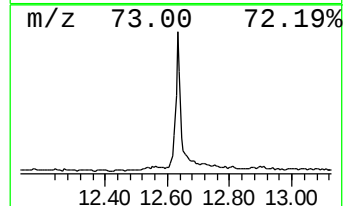
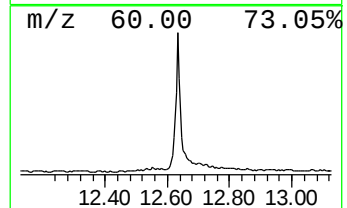
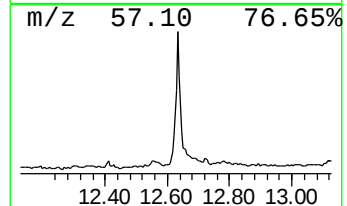
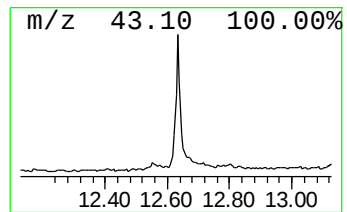
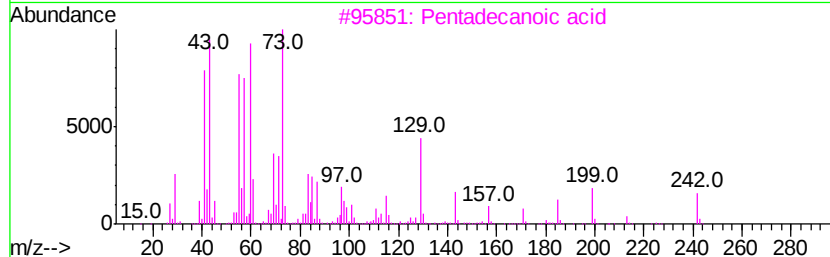
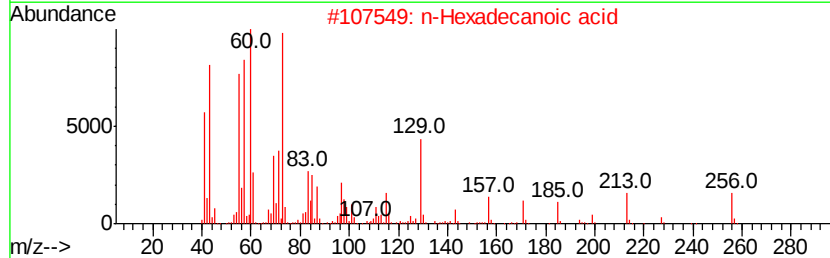
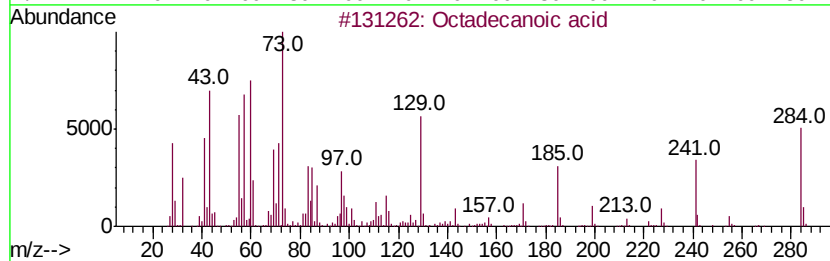
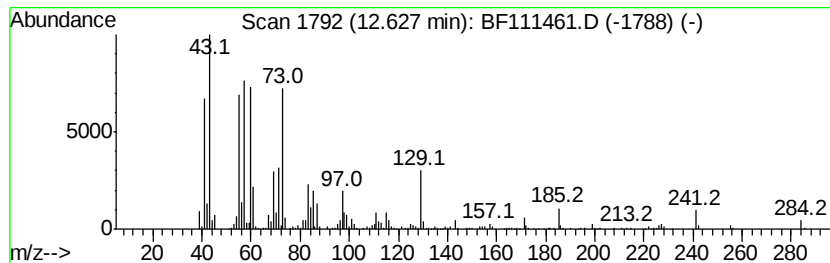
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	20.95 ng	1381970	Chrysene-d12	13.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4		Tridecanoic acid	214	C13H26O2	000638-53-9	78
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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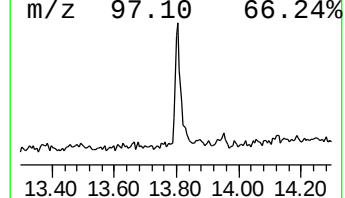
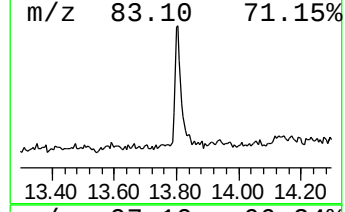
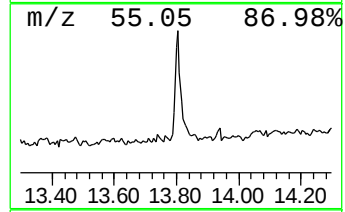
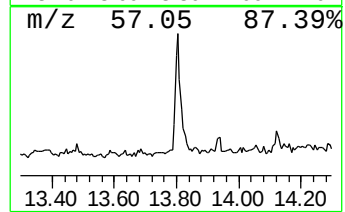
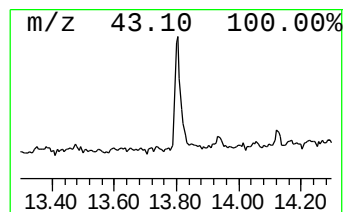
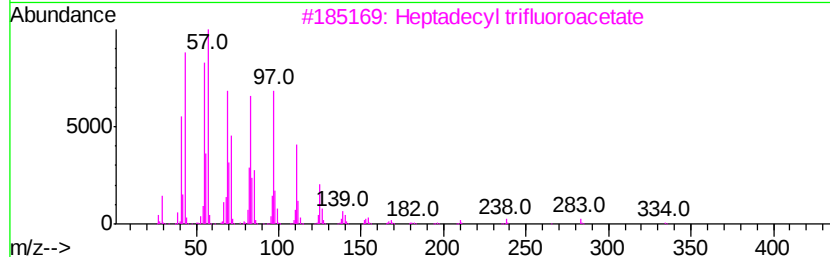
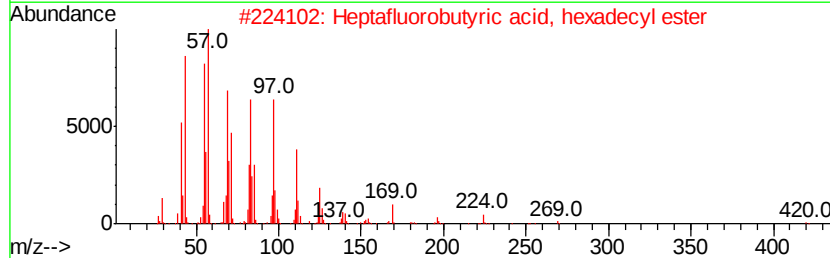
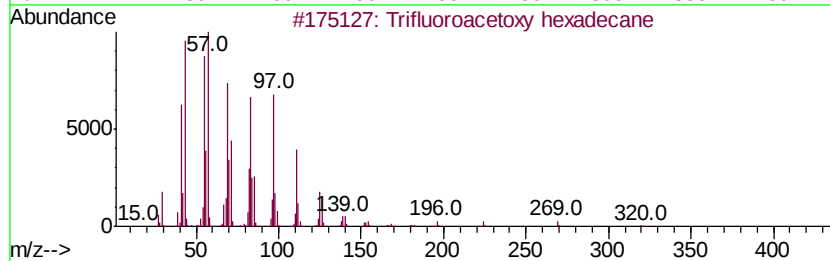
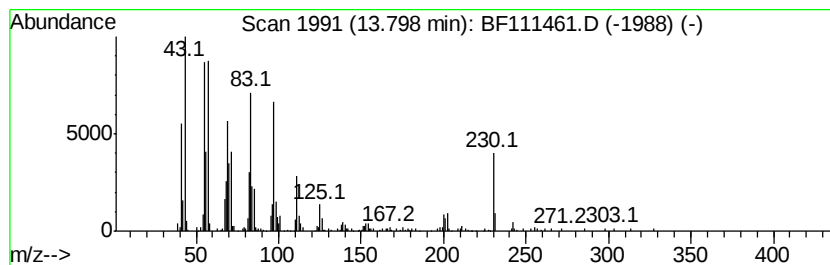
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.80	6.28 ng	414308	Chrysene-d12	13.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4	Cyclopentadecane	210	C15H30	000295-48-7	92
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121518\
Data File : BF111461.D
Acq On : 15 Dec 2018 11:50
Operator : JU/SJ
Sample : J6208-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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...	5.00	3.2	ng	169121	1	6.79	1058830	20.0
unknown6.57	6.57	63.5	ng	3361250	1	6.79	1058830	20.0
n-Hexadecanoic acid	11.85	26.4	ng	1722450	4	11.31	1305690	20.0
Octadecanoic acid	12.63	20.9	ng	1381970	5	13.95	1319410	20.0
Trifluoroacetoxy ...	13.80	6.3	ng	414308	5	13.95	1319410	20.0