

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
 Data File : BF111293.D
 Acq On : 11 Dec 2018 23:17
 Operator : JU/SJ
 Sample : J6157-11
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-6-TOTAL

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-BF120818.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	3.781	283	288	292	rBV2	28280	43384	2.34%	0.256%
2	4.022	322	329	340	rBV	47224	66825	3.60%	0.394%
3	4.963	484	489	490	rBV2	84458	86578	4.66%	0.511%
4	4.981	490	492	501	rVB	92945	96162	5.18%	0.567%
5	5.398	560	563	572	rBV	273685	266330	14.34%	1.571%
6	5.739	618	621	626	rVB	32637	27796	1.50%	0.164%
7	5.916	648	651	655	rVB	70741	56345	3.03%	0.332%
8	6.428	733	738	749	rBV2	702917	773360	41.65%	4.561%
9	6.557	757	760	765	rBV	451749	372393	20.06%	2.196%
10	6.792	797	800	804	rBV	1729740	1399259	75.36%	8.251%
11	6.857	809	811	816	rVV	50998	44365	2.39%	0.262%
12	6.951	823	827	831	rVB	452406	397111	21.39%	2.342%
13	7.345	891	894	902	rBV	348348	288262	15.53%	1.700%
14	7.575	929	933	937	rBV	48026	39739	2.14%	0.234%
15	8.075	1014	1018	1022	rBV	2116086	1782470	96.00%	10.511%
16	8.386	1069	1071	1079	rVB2	19158	24979	1.35%	0.147%
17	9.151	1197	1201	1205	rBV	687088	525323	28.29%	3.098%
18	9.545	1264	1268	1271	rBV	798857	594208	32.00%	3.504%
19	9.727	1295	1299	1304	rVB3	17656	25590	1.38%	0.151%
20	9.833	1313	1317	1320	rBV	2057772	1844250	99.33%	10.876%
21	10.245	1384	1387	1389	rBV	26727	21325	1.15%	0.126%
22	10.610	1446	1449	1454	rBV	221793	202432	10.90%	1.194%
23	10.745	1469	1472	1479	rVB4	19832	27089	1.46%	0.160%
24	11.316	1565	1569	1572	rBV	1973745	1856654	100.00%	10.949%
25	11.380	1576	1580	1584	rVB4	14061	21748	1.17%	0.128%
26	11.551	1604	1609	1615	rBV8	10711	22903	1.23%	0.135%
27	11.845	1656	1659	1670	rBV	586984	606682	32.68%	3.578%
28	12.415	1752	1756	1759	rVB4	26111	31033	1.67%	0.183%
29	12.533	1771	1776	1778	rBV4	27744	38192	2.06%	0.225%
30	12.633	1789	1793	1802	rBV	247351	265105	14.28%	1.563%
31	12.898	1834	1838	1841	rBV	475226	398826	21.48%	2.352%
32	12.933	1841	1844	1847	rVB	384829	317206	17.08%	1.871%
33	13.368	1915	1918	1925	rVB8	13320	24336	1.31%	0.144%
34	13.804	1987	1992	2001	rBV2	450373	681016	36.68%	4.016%

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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	13.951	2013	2017	2020	rBV	1837797	1655570	89.17%	9.763%
36	14.133	2045	2048	2052	rBV2	38089	46659	2.51%	0.275%
37	14.439	2096	2100	2106	rBV3	64963	101515	5.47%	0.599%
38	14.739	2148	2151	2154	rVB	75250	63587	3.42%	0.375%
39	15.068	2204	2207	2210	rBV	78177	80823	4.35%	0.477%
40	15.386	2256	2261	2266	rBV	1206760	1380435	74.35%	8.140%
41	15.439	2266	2270	2274	rVB	69850	89829	4.84%	0.530%
42	15.862	2337	2342	2347	rBV	63802	90920	4.90%	0.536%
43	15.915	2347	2351	2360	rBV10	51385	156445	8.43%	0.923%
44	16.351	2422	2425	2426	rBV2	24220	22631	1.22%	0.133%

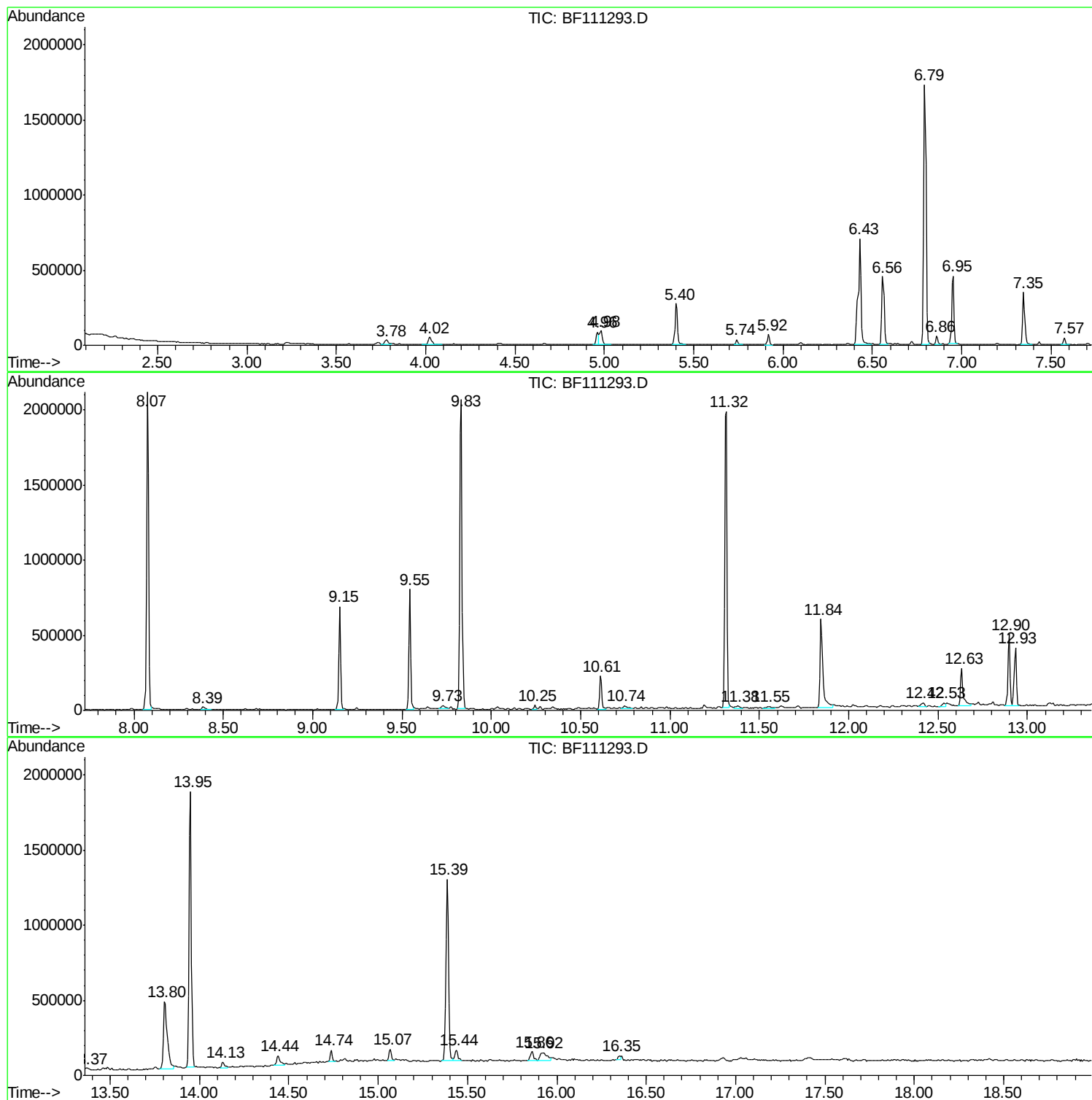
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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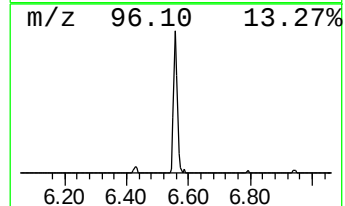
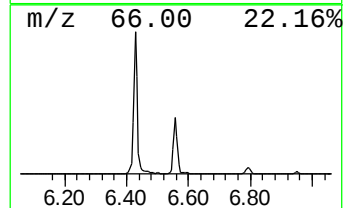
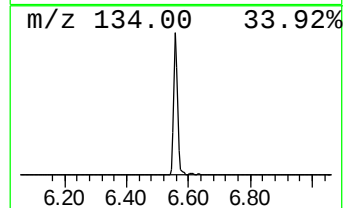
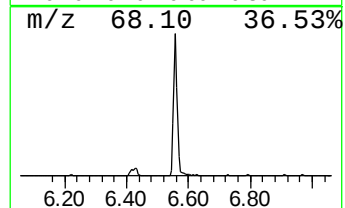
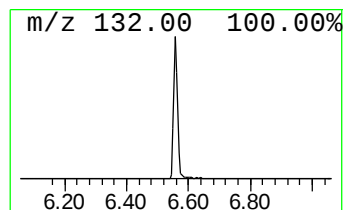
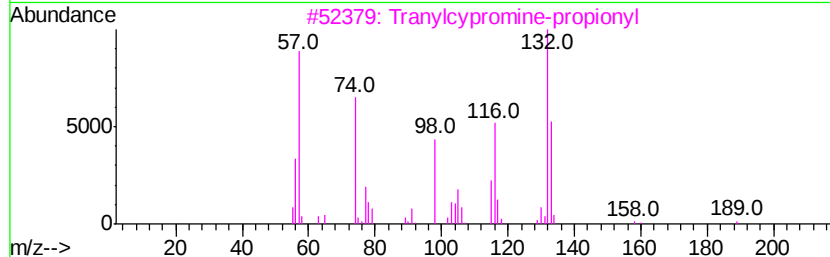
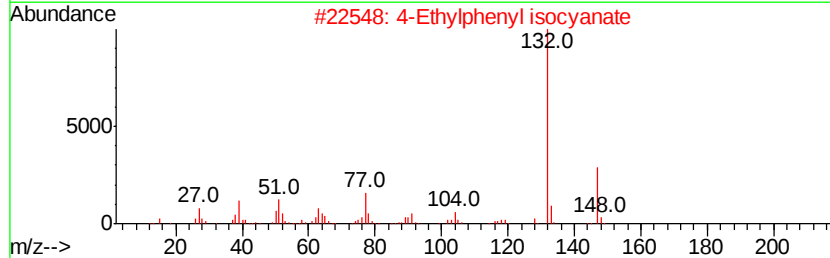
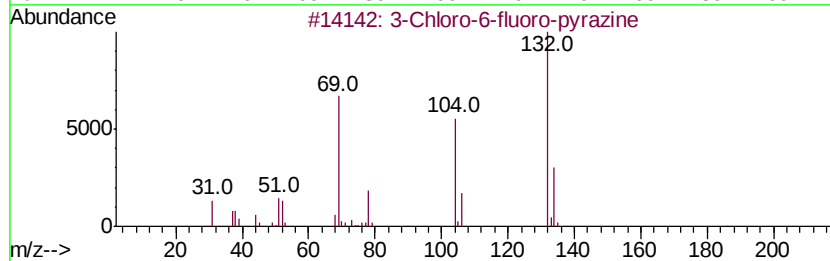
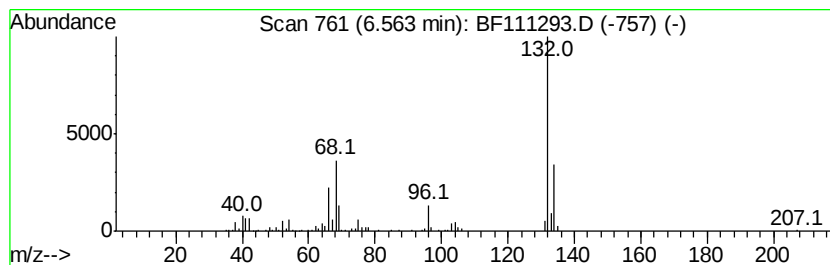
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.56 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	5.32 ng	372393	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			4-Ethylphenyl isocyanate	147	C9H9NO	023138-50-3	10
3			Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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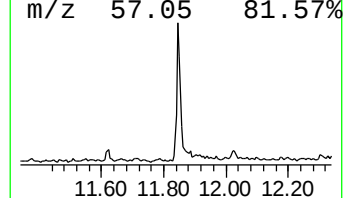
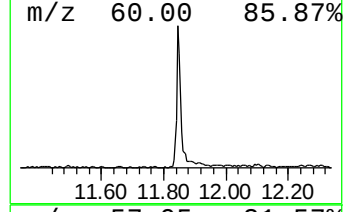
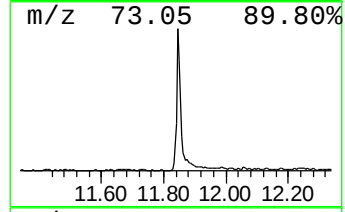
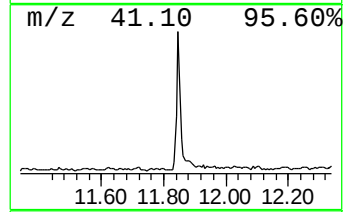
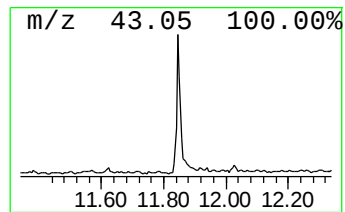
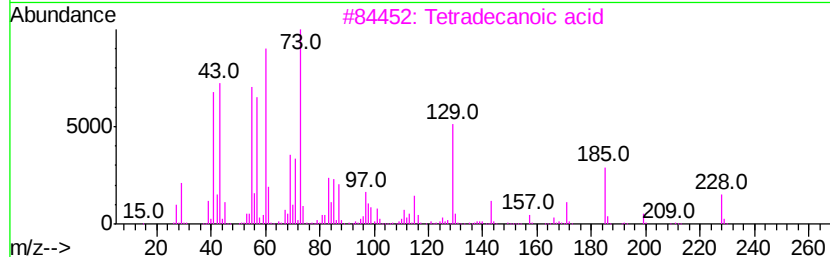
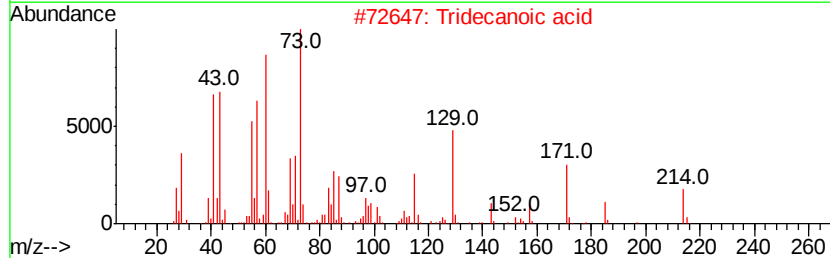
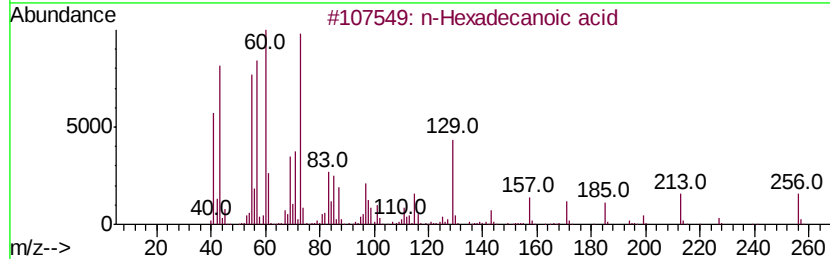
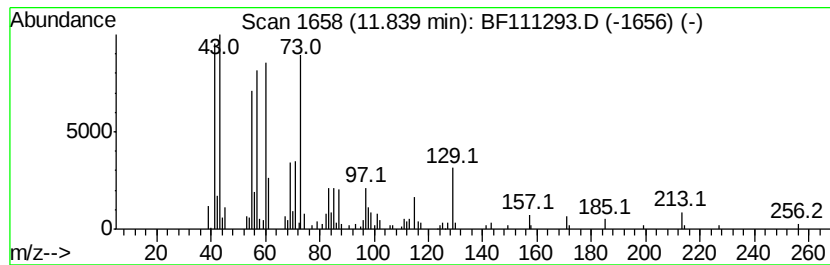
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	6.54 ng	606682	Phenanthrene-d10	11.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5		Undecanoic acid	186	C11H22O2	000112-37-8	81



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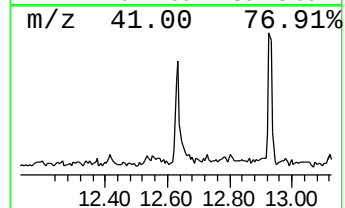
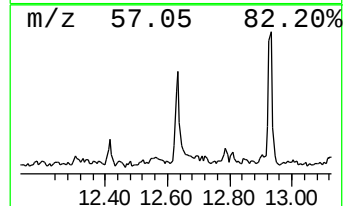
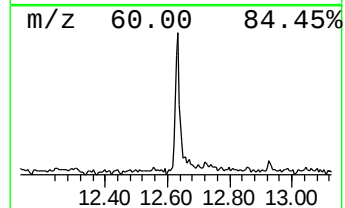
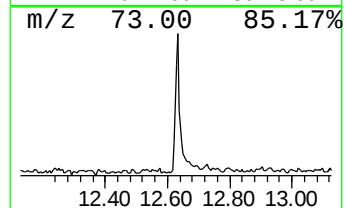
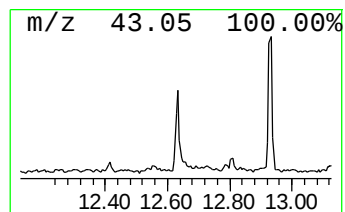
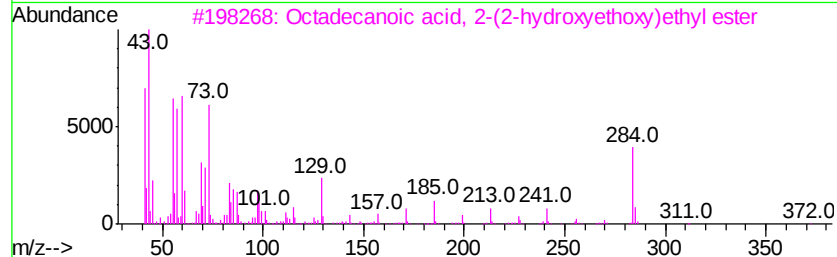
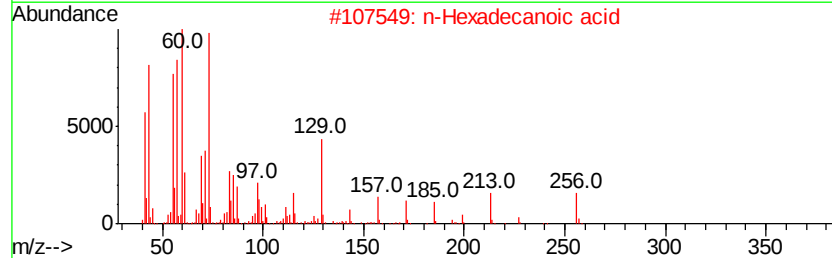
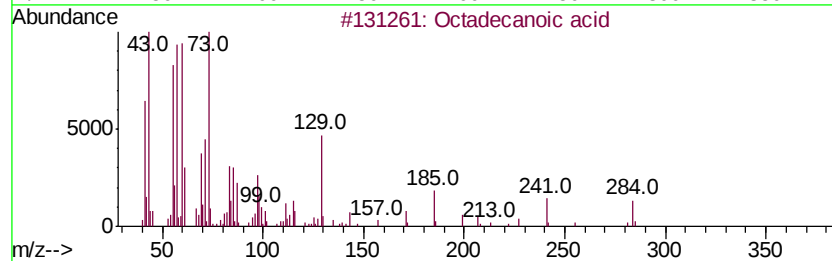
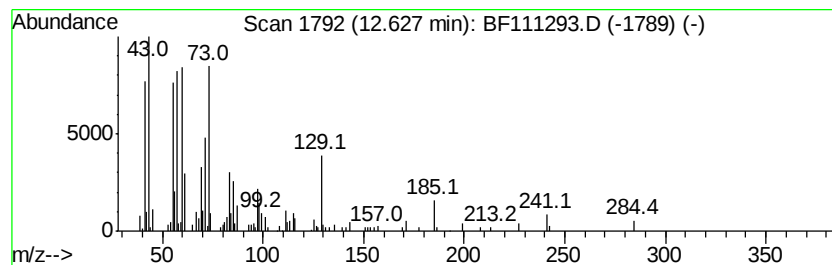
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	3.20 ng	265105	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	90
3		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	59
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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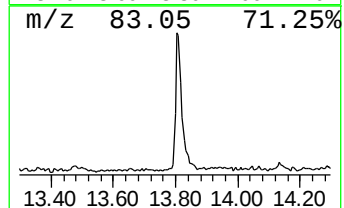
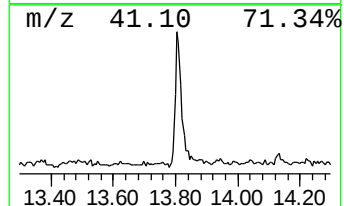
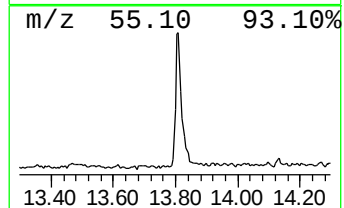
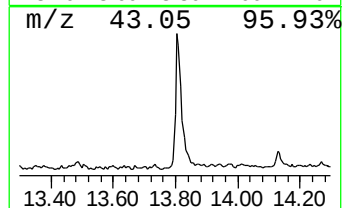
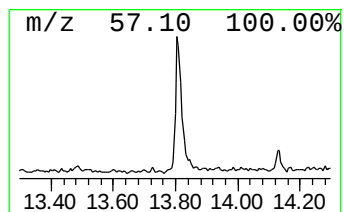
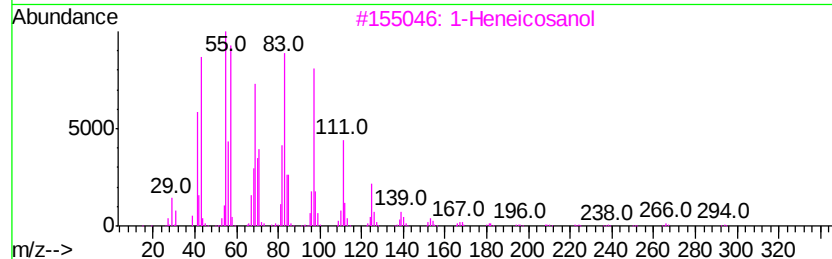
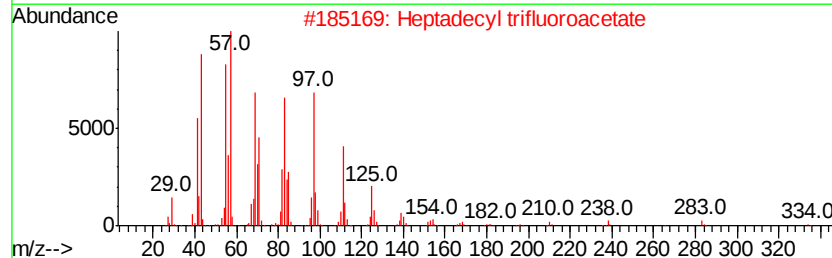
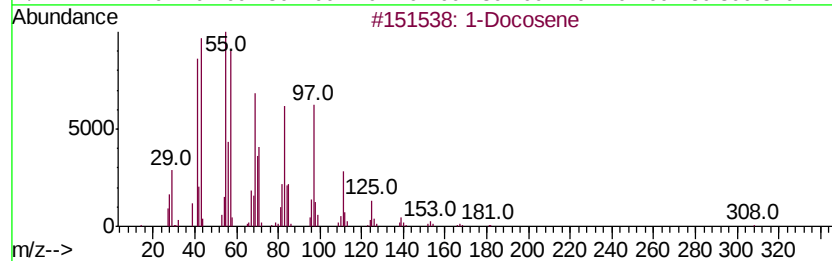
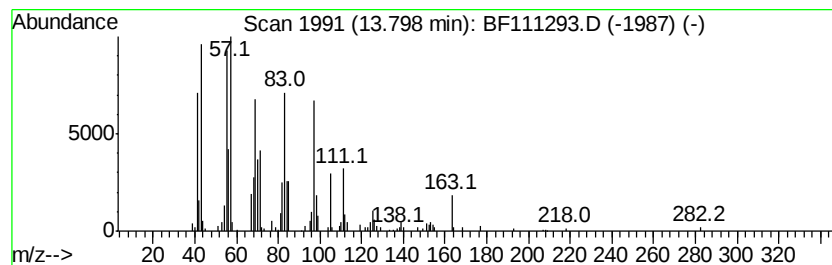
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Docosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	8.23 ng	681016	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	94
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91



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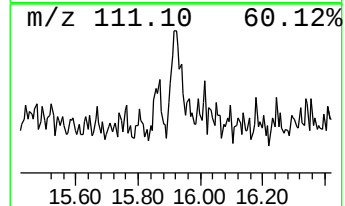
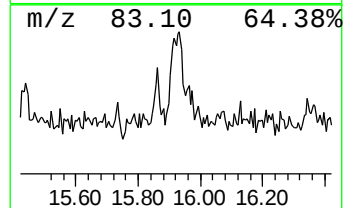
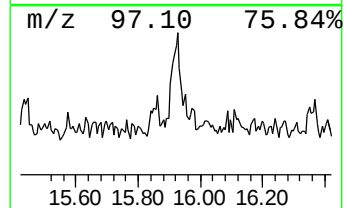
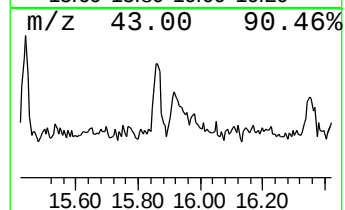
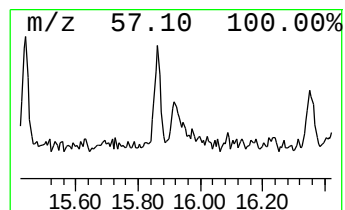
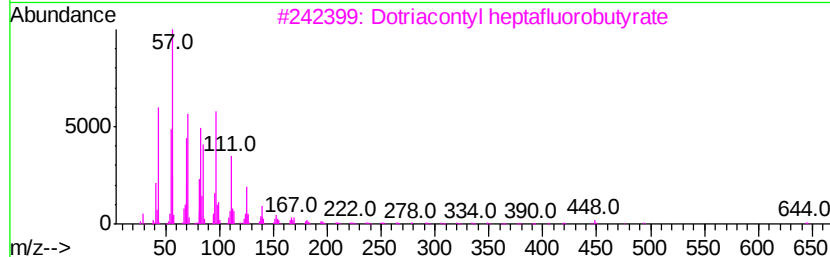
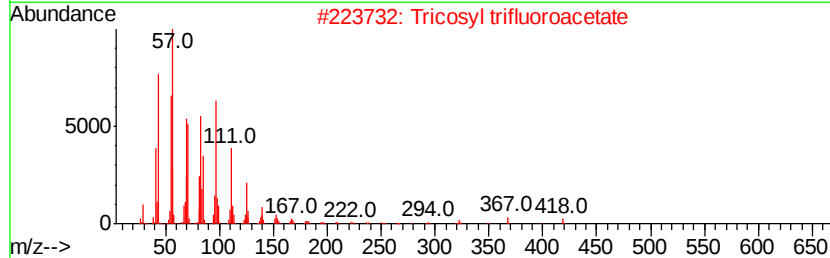
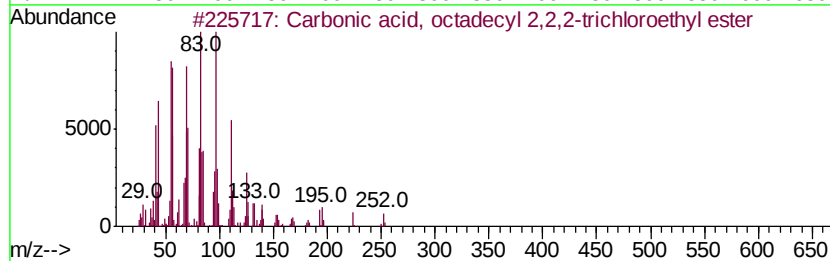
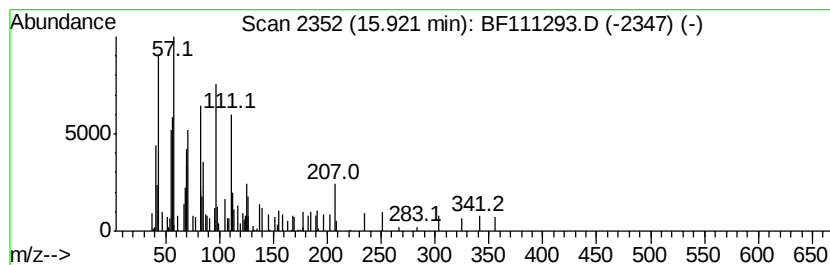
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Carbonic acid, octadecyl 2,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	2.27 ng	156445	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	52
2		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	49
3		Dotriacontyl heptafluorobutyrate	662	C36H65F7O2	1000351-84-2	49
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	49
5		Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
Data File : BF111293.D
Acq On : 11 Dec 2018 23:17
Operator : JU/SJ
Sample : J6157-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-6-TOTAL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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
unknown6.56	6.56	5.3	ng	372393	1	6.79	1399260	20.0
n-Hexadecanoic acid	11.84	6.5	ng	606682	4	11.32	1856650	20.0
Octadecanoic acid	12.63	3.2	ng	265105	5	13.95	1655570	20.0
1-Docosene	13.80	8.2	ng	681016	5	13.95	1655570	20.0
Carbonic acid, oc...	15.92	2.3	ng	156445	6	15.39	1380440	20.0