

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
 Data File : BF121061.D
 Acq On : 28 Jul 2020 10:48
 Operator : JU/CG
 Sample : L3435-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1

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-BF071620.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	5.428	563	568	571	rBV	3326503	3863074	72.62%	10.729%
2	6.445	735	741	744	rBV	3274453	3797149	71.38%	10.546%
3	6.640	772	774	784	rBV	39490	56342	1.06%	0.156%
4	6.810	799	803	806	rBV	1125744	864330	16.25%	2.401%
5	7.375	894	899	902	rBV	2537398	2640850	49.64%	7.335%
6	8.092	1017	1021	1027	rBV	1333665	1127431	21.19%	3.131%
7	9.169	1199	1204	1215	rBV	3907362	4691654	88.19%	13.030%
8	9.286	1222	1224	1239	rVB2	47875	76720	1.44%	0.213%
9	9.563	1267	1271	1284	rBV	539293	491848	9.25%	1.366%
10	9.845	1315	1319	1333	rBV	1428828	1339502	25.18%	3.720%
11	10.639	1448	1454	1467	rBV	2484043	3207229	60.29%	8.908%
12	10.745	1469	1472	1477	rVB	50908	69258	1.30%	0.192%
13	11.328	1567	1571	1577	rBV	1482822	1484206	27.90%	4.122%
14	11.722	1634	1638	1642	rBV	51122	54022	1.02%	0.150%
15	11.863	1653	1662	1666	rBV	212021	218145	4.10%	0.606%
16	12.304	1734	1737	1741	rVB	65405	61902	1.16%	0.172%
17	12.516	1769	1773	1776	rBV	58931	62517	1.18%	0.174%
18	12.922	1836	1842	1845	rBV2	4316737	5319928	100.00%	14.775%
19	13.145	1874	1880	1886	rBV2	56279	79833	1.50%	0.222%
20	13.486	1933	1938	1941	rBV2	76534	83596	1.57%	0.232%
21	13.816	1990	1994	2011	rBV	842625	1319529	24.80%	3.665%
22	13.969	2015	2020	2030	rVV	1553948	1633905	30.71%	4.538%
23	14.133	2045	2048	2056	rBV	104775	112964	2.12%	0.314%
24	14.439	2095	2100	2111	rBV3	128575	263872	4.96%	0.733%
25	14.739	2148	2151	2155	rBV	94245	97642	1.84%	0.271%
26	15.074	2203	2208	2211	rBV	164930	184802	3.47%	0.513%
27	15.415	2260	2266	2279	rBV	1199101	1749376	32.88%	4.859%
28	15.868	2338	2343	2348	rBV	100145	150493	2.83%	0.418%
29	15.927	2348	2353	2361	rBV2	133841	353726	6.65%	0.982%
30	16.357	2420	2426	2431	rBV3	55126	121054	2.28%	0.336%
31	16.945	2521	2526	2533	rVB2	26965	53601	1.01%	0.149%
32	17.051	2536	2544	2553	rBV8	39782	167537	3.15%	0.465%
33	17.427	2600	2608	2623	rBV8	56739	207276	3.90%	0.576%

LSC Area Percent Report

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
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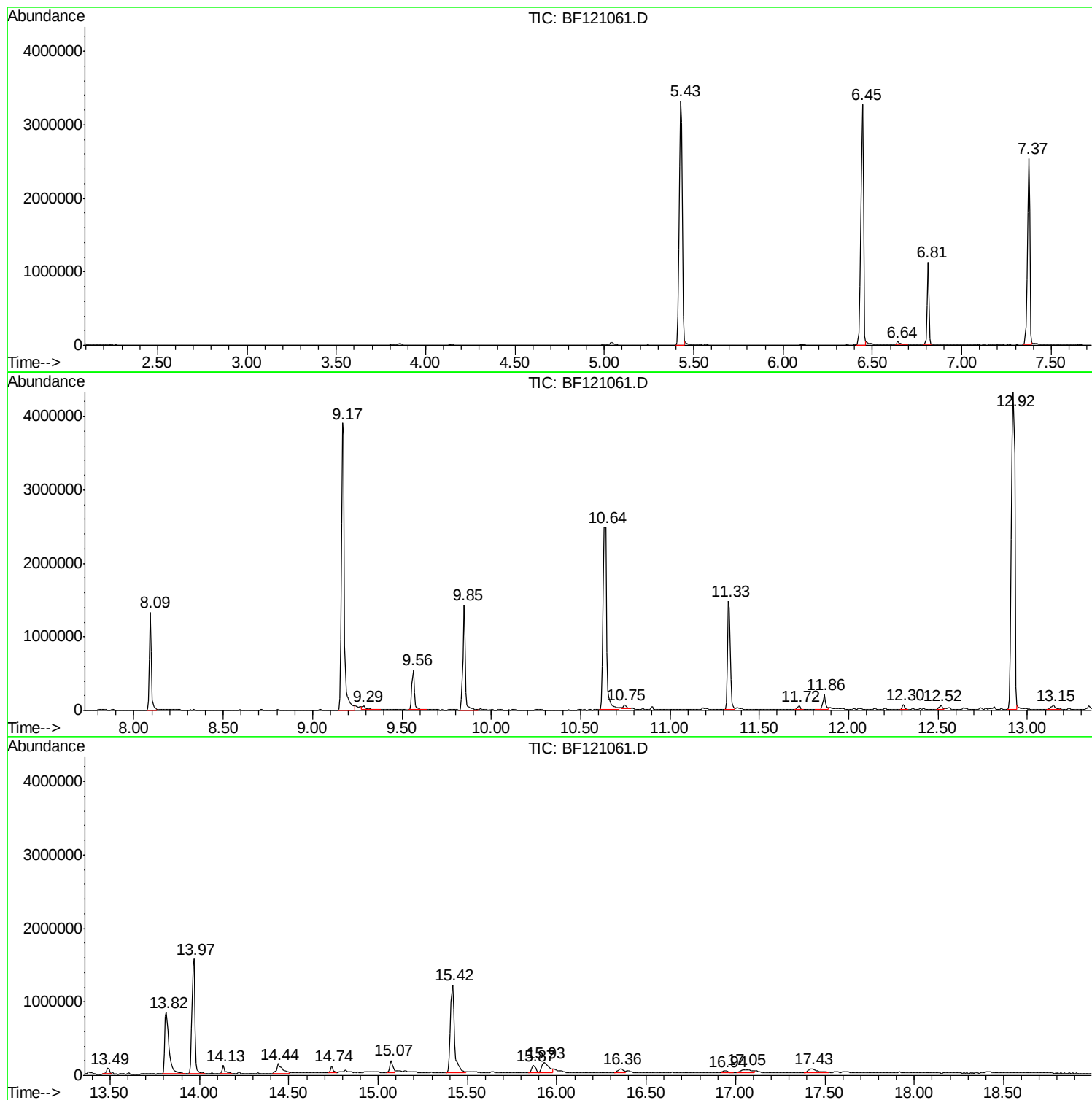
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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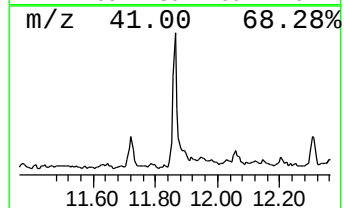
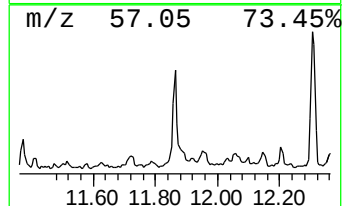
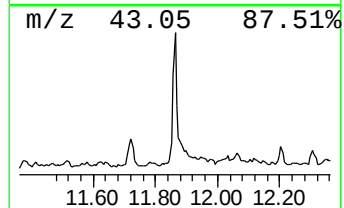
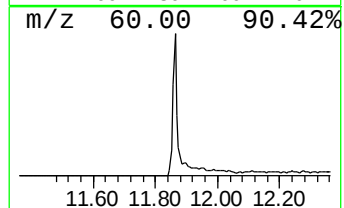
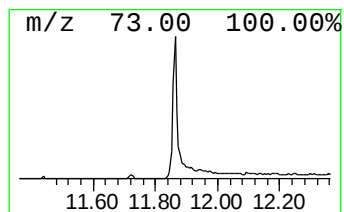
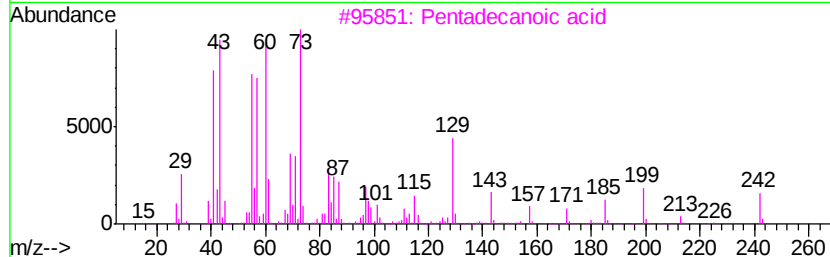
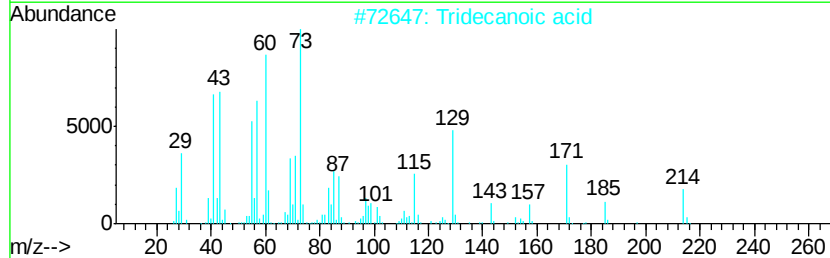
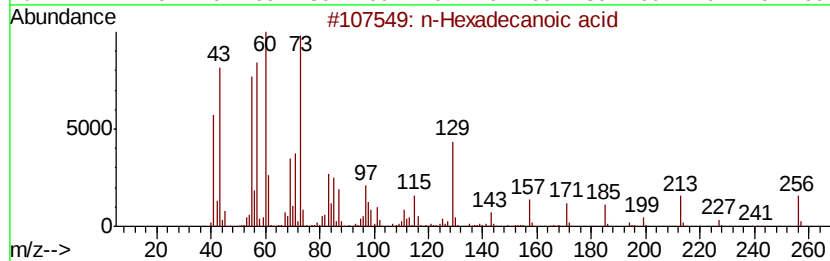
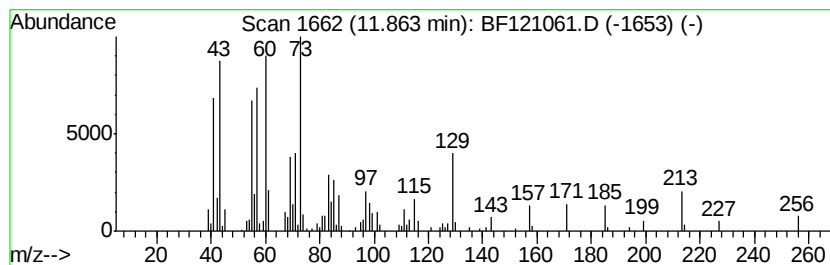
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.86	2.94 ng	218145	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	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



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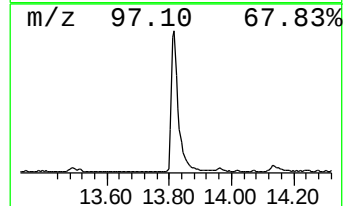
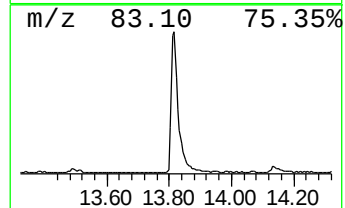
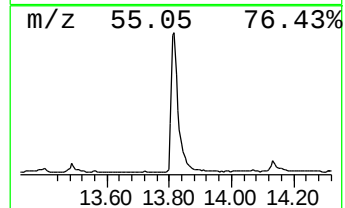
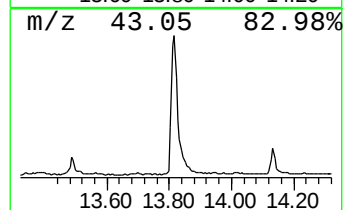
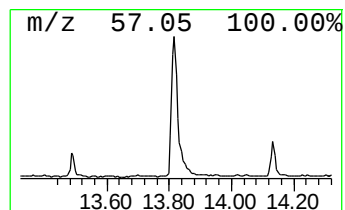
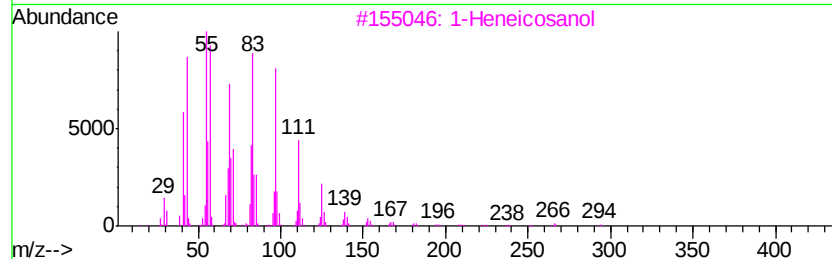
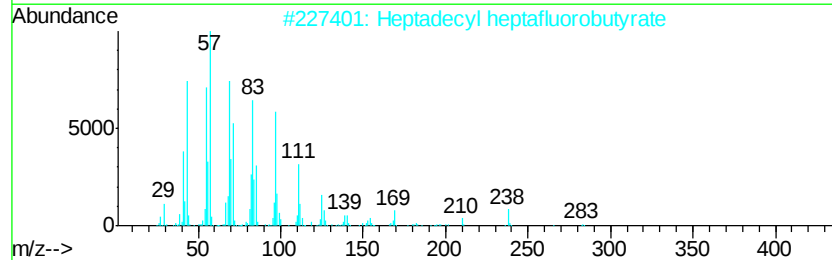
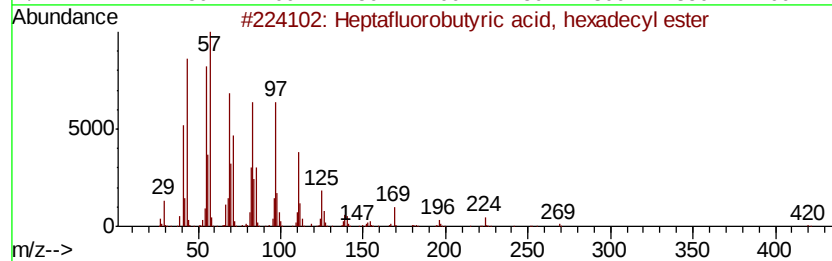
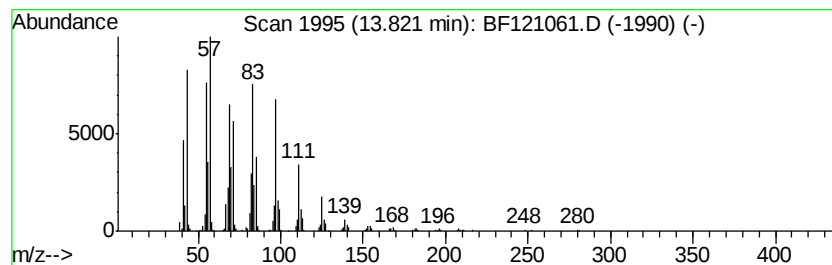
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptafluorobutyric acid, he... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	16.15 ng	1319530	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2		Heptadecyl heptafluorobutyrat	452	C21H35F7O2	959085-66-6	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		Behenic alcohol	326	C22H46O	000661-19-8	91
5		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91



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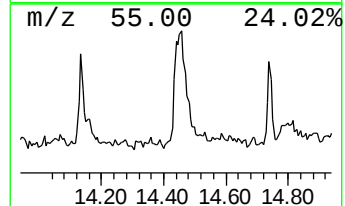
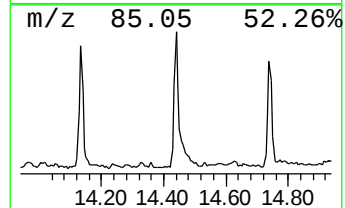
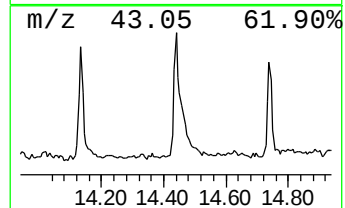
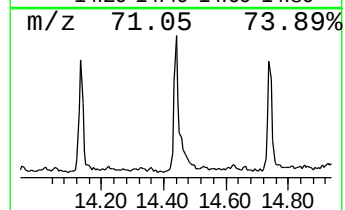
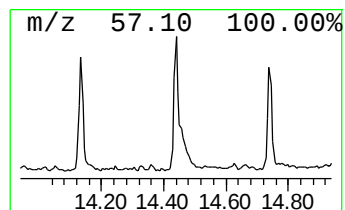
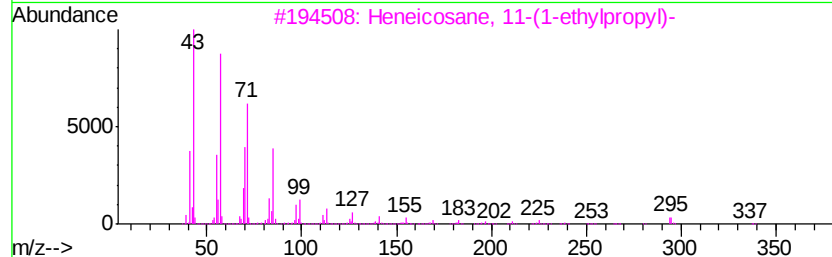
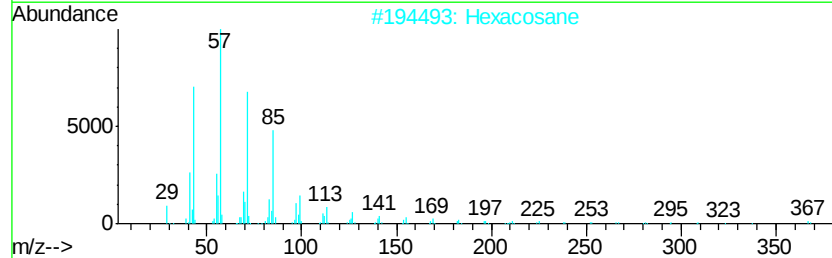
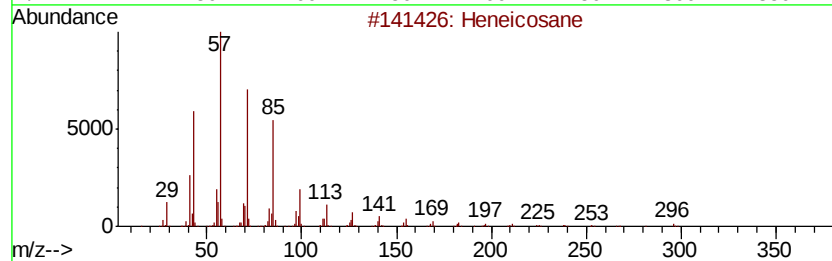
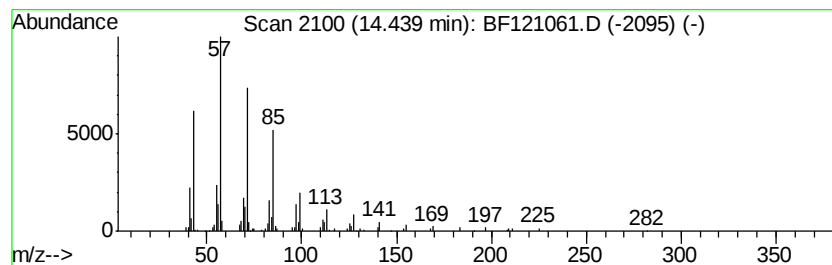
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	3.23 ng	263872	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Heneicosane, 11-(1-ethylpropyl)-		366	C26H54	055282-11-6	91
4	Hentriacontane		437	C31H64	000630-04-6	91
5	Octacosane		394	C28H58	000630-02-4	90



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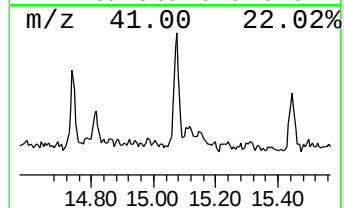
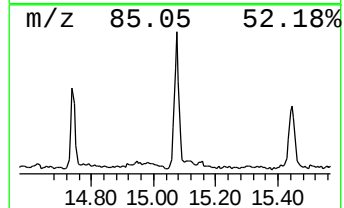
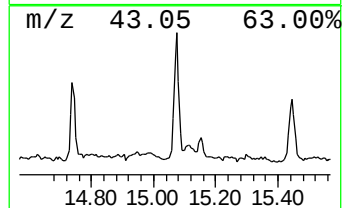
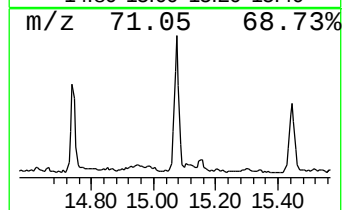
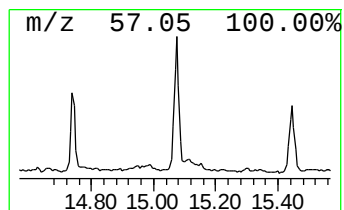
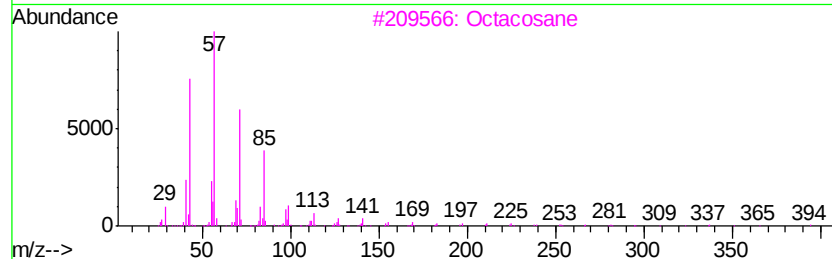
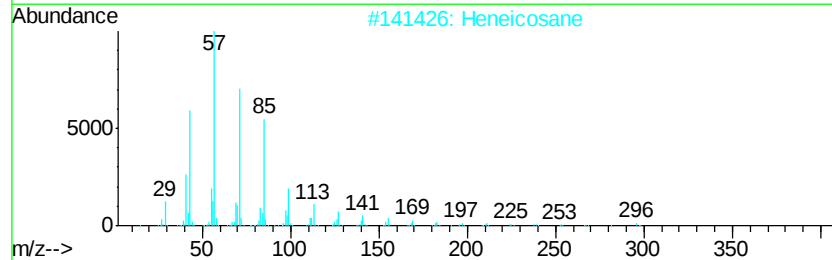
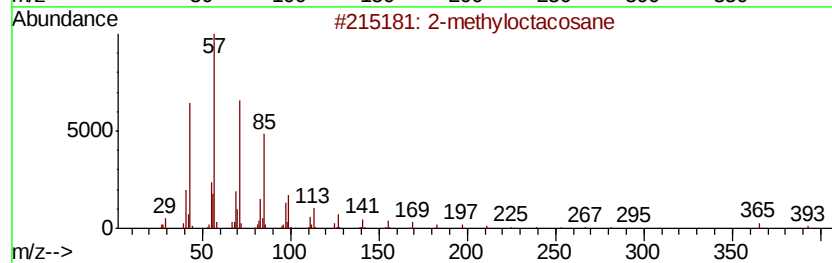
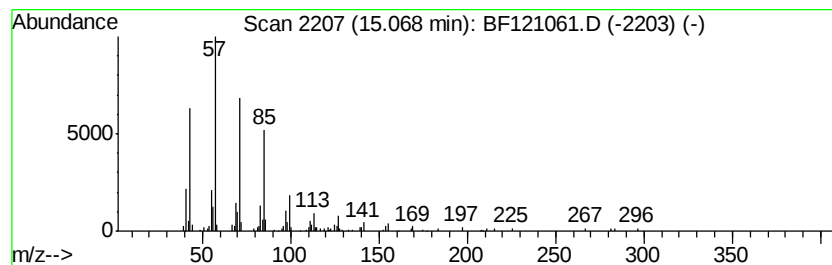
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.11 ng	184802	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	90
4		Hexacosane	366	C26H54	000630-01-3	87
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86



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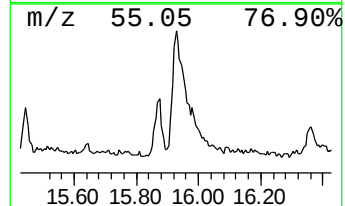
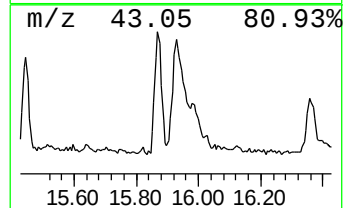
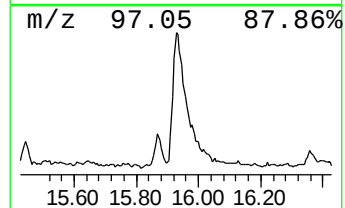
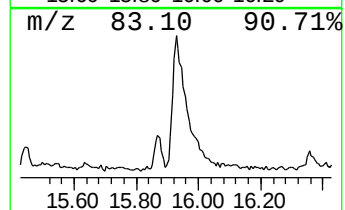
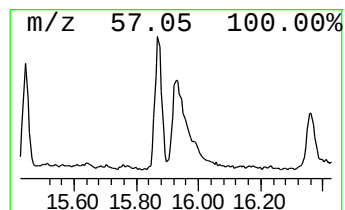
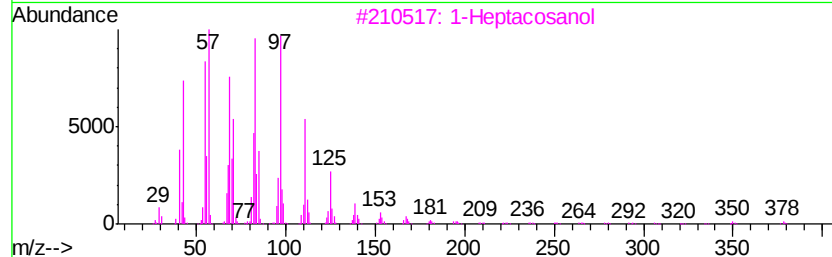
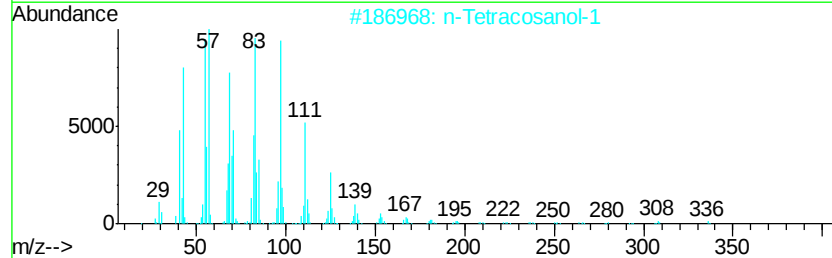
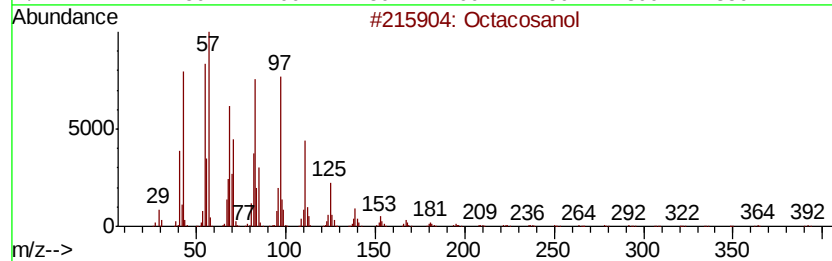
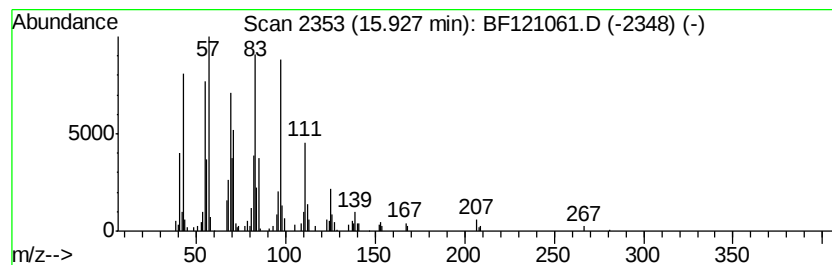
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	4.04 ng	353726	Perylene-d12	15.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosanol	410	C28H58O	000557-61-9	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3		1-Heptacosanol	396	C27H56O	002004-39-9	94
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



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ALS Vial : 4 Sample Multiplier: 1

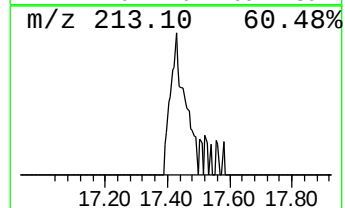
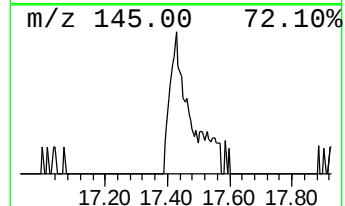
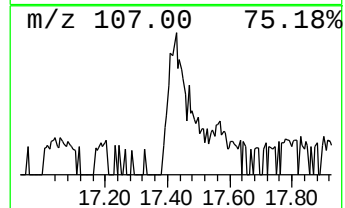
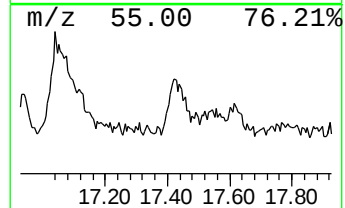
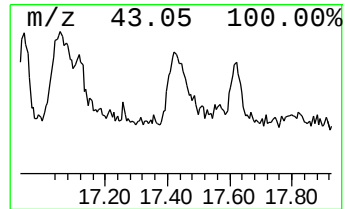
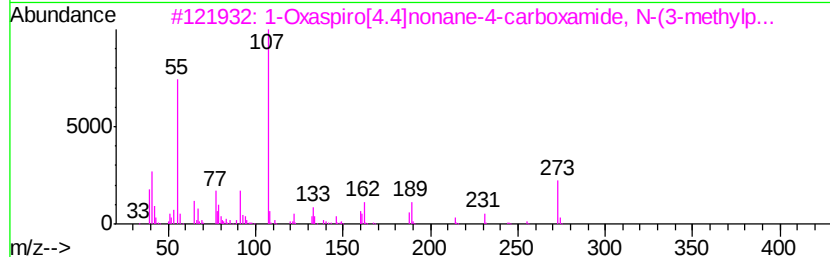
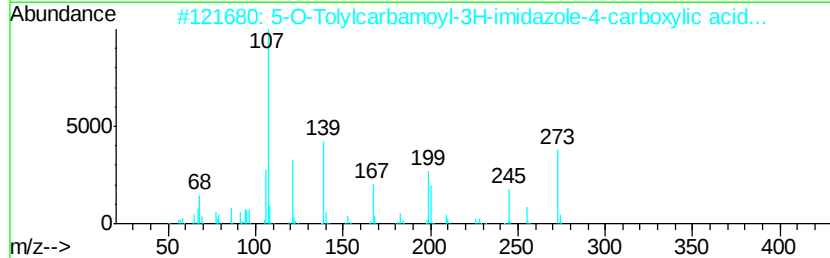
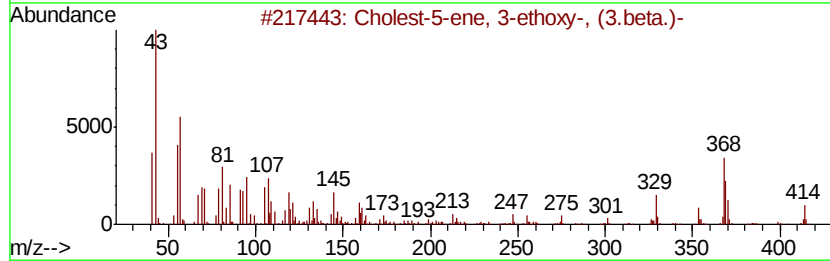
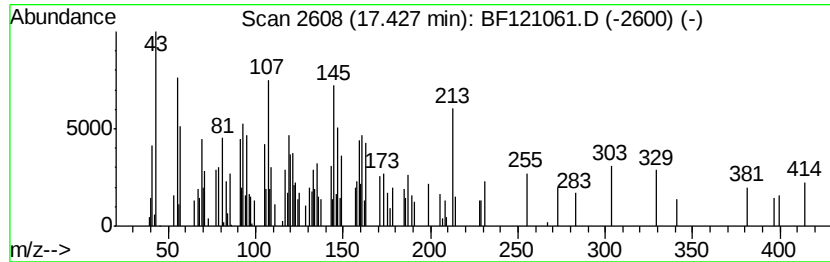
Instrument :
BNA_F
ClientSampleId :
SP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown17.43 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.43	2.37 ng	207276	Perylene-d12	15.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cholest-5-ene, 3-ethoxy-, (3.beta...	414 C29H50O	000986-19-6 18
2		5-O-Tolylcarbamoyl-3H-imidazole-...	273 C14H15N3O3	313251-31-9 14
3		1-Oxaspiro[4.4]nonane-4-carboxam...	273 C16H19N3O3	1000319-97-0 14
4		2,6-Bis(3-(pyrid-2-yl)-2-azaprop...	319 C19H21N5	090719-79-2 14
5		5-Cholene, 3,24-dihydroxy-	360 C24H40O2	1000251-69-2 10



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072820\
Data File : BF121061.D
Acq On : 28 Jul 2020 10:48
Operator : JU/CG
Sample : L3435-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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
n-Hexadecanoic acid	11.86	2.9 ng		218145	4	11.33	1484210	20.0
Heptafluorobutyri...	13.82	16.1 ng		1319530	5	13.97	1633910	20.0
Heneicosane	14.44	3.2 ng		263872	5	13.97	1633910	20.0
2-methyloctacosane	15.07	2.1 ng		184802	6	15.42	1749380	20.0
Octacosanol	15.93	4.0 ng		353726	6	15.42	1749380	20.0
unknown17.43	17.43	2.4 ng		207276	6	15.42	1749380	20.0