

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020124\
 Data File : BF137233.D
 Acq On : 01 Feb 2024 15:52
 Operator : CG\JU
 Sample : P1307-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-614-COMP-01

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-BF013024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137233.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	14	18	26	rVB	13128	18362	1.36%	0.177%
2	5.028	495	500	508	rVB	29443	38453	2.85%	0.371%
3	5.422	563	567	587	rBV	1215365	1214643	90.17%	11.704%
4	6.422	733	737	757	rBV	1232807	1230440	91.35%	11.856%
5	6.792	796	800	808	rBV	398959	365420	27.13%	3.521%
6	7.351	891	895	907	rBV	821362	771298	57.26%	7.432%
7	8.069	1013	1017	1032	rBV	541058	481930	35.78%	4.644%
8	9.145	1196	1200	1203	rBV	1678982	1347014	100.00%	12.979%
9	9.822	1311	1315	1320	rBV	631082	523600	38.87%	5.045%
10	9.928	1328	1333	1338	rVB	19597	24905	1.85%	0.240%
11	10.610	1446	1449	1461	rBV	893117	809352	60.08%	7.799%
12	11.316	1565	1569	1571	rBV	497272	456232	33.87%	4.396%
13	11.339	1571	1573	1579	rVB	54625	51982	3.86%	0.501%
14	11.857	1657	1661	1671	rBV2	182552	203989	15.14%	1.966%
15	12.527	1772	1775	1781	rBV	129819	130071	9.66%	1.253%
16	12.645	1792	1795	1804	rBV2	53920	74433	5.53%	0.717%
17	12.757	1808	1814	1819	rBV	117791	131455	9.76%	1.267%
18	12.910	1836	1840	1849	rBV	1152259	1038926	77.13%	10.011%
19	13.092	1868	1871	1875	rVB	15901	16181	1.20%	0.156%
20	13.157	1875	1882	1885	rBV2	17839	18904	1.40%	0.182%
21	13.827	1991	1996	2007	rBV4	62171	101797	7.56%	0.981%
22	13.968	2013	2020	2023	rBV2	432818	494289	36.70%	4.763%
23	13.992	2023	2024	2031	rVB	67283	51281	3.81%	0.494%
24	14.463	2099	2104	2106	rBV3	19144	29436	2.19%	0.284%
25	14.851	2164	2170	2174	rBV	46581	58413	4.34%	0.563%
26	15.010	2193	2197	2201	rBV	58257	93035	6.91%	0.896%
27	15.121	2212	2216	2221	rVB2	21085	24484	1.82%	0.236%
28	15.321	2245	2250	2256	rVB	32988	44336	3.29%	0.427%
29	15.380	2256	2260	2266	rBV	39758	52536	3.90%	0.506%
30	15.445	2266	2271	2280	rBV	296313	389085	28.89%	3.749%
31	16.033	2365	2371	2375	rBV7	8415	20126	1.49%	0.194%
32	16.933	2519	2524	2532	rVB4	12145	26525	1.97%	0.256%
33	17.133	2551	2558	2564	rBV10	8172	21401	1.59%	0.206%
34	17.380	2594	2600	2607	rVB3	10598	23886	1.77%	0.230%

Sum of corrected areas: 10378220

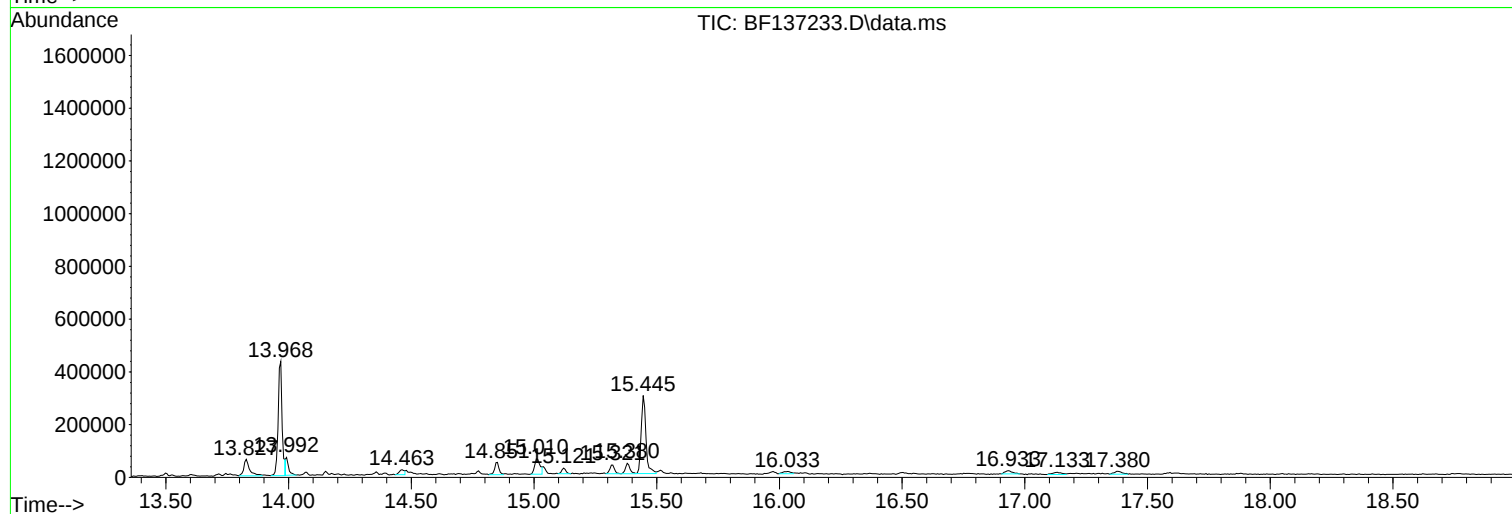
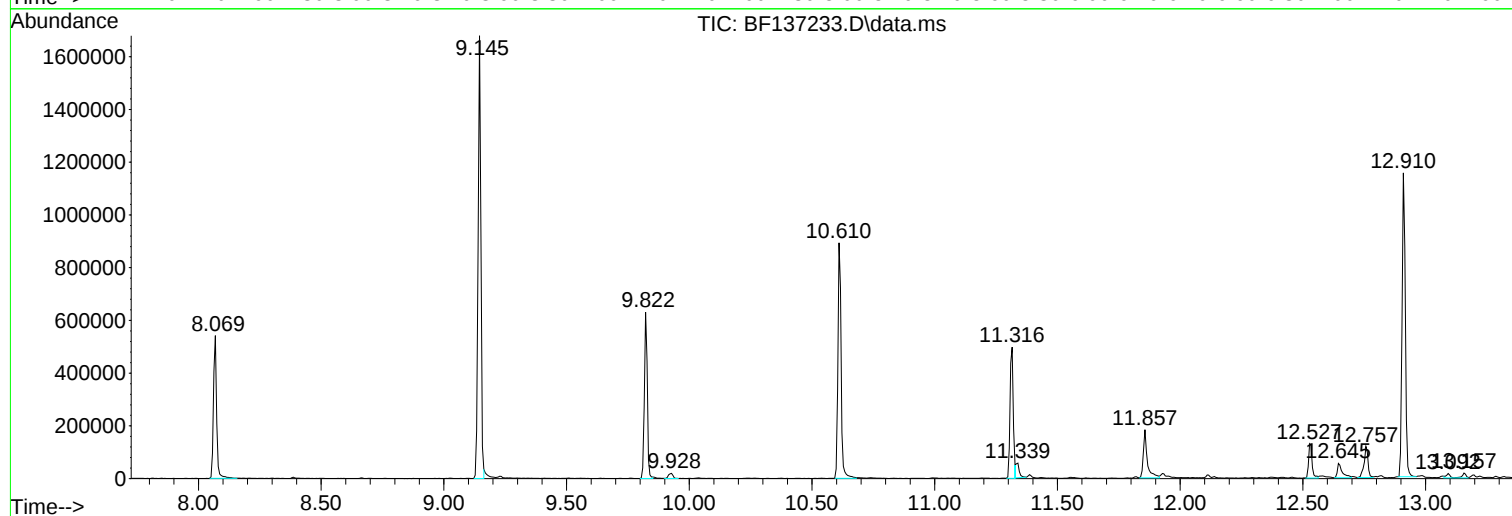
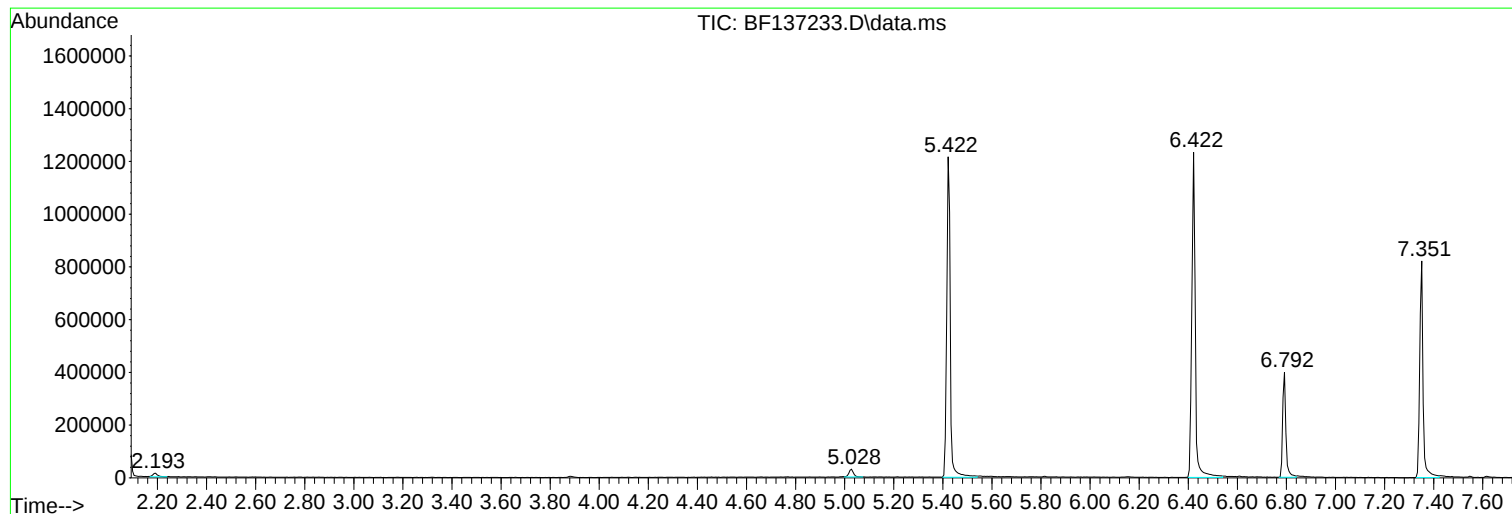
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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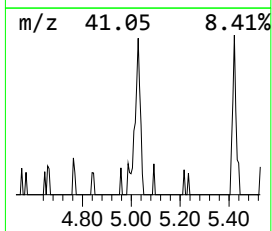
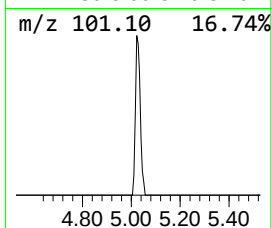
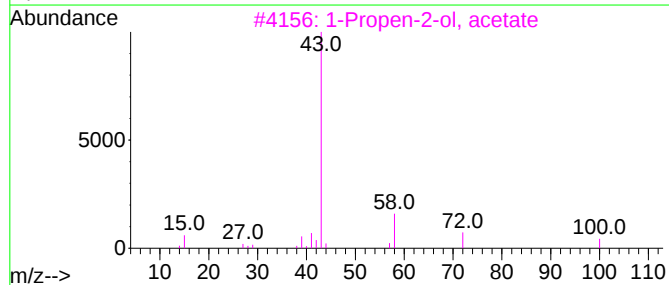
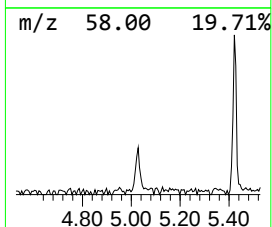
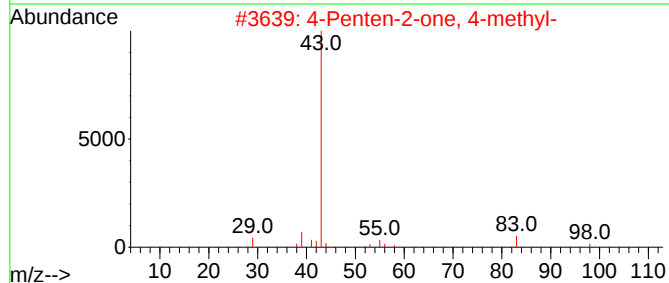
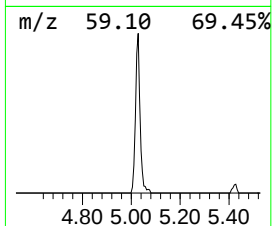
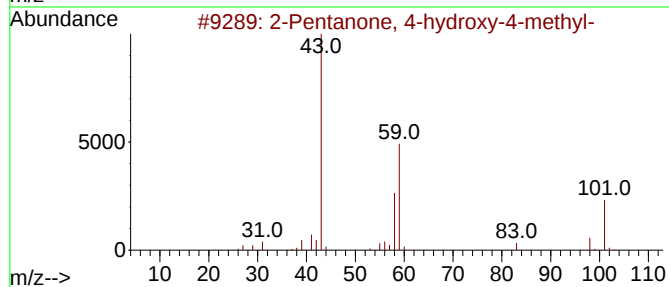
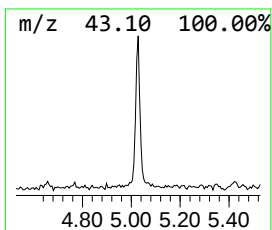
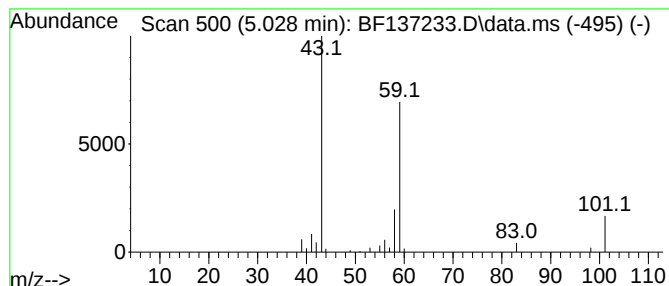
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	2.10 ng	38453	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	14		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9		
5	3-Octanol	130	C8H18O	000589-98-0	9		



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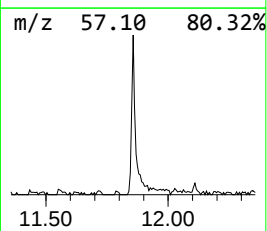
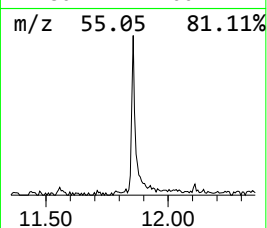
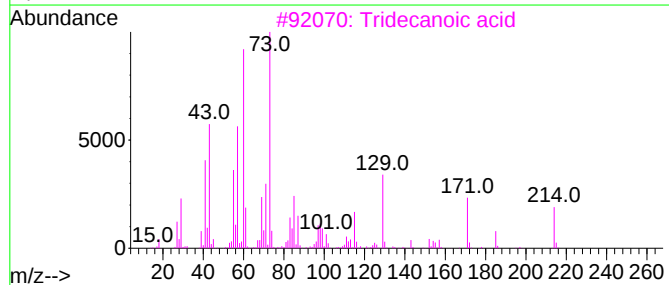
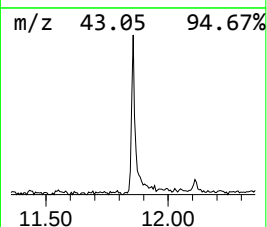
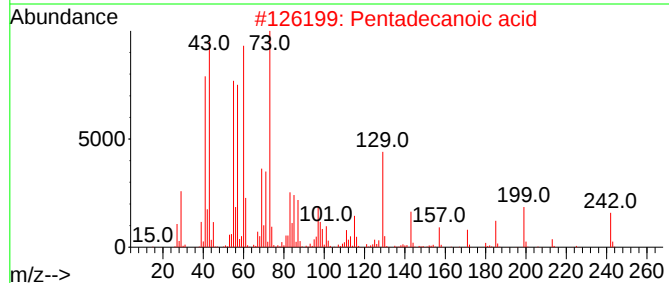
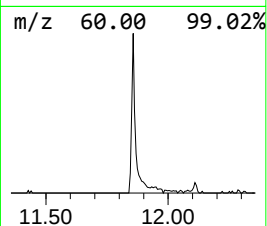
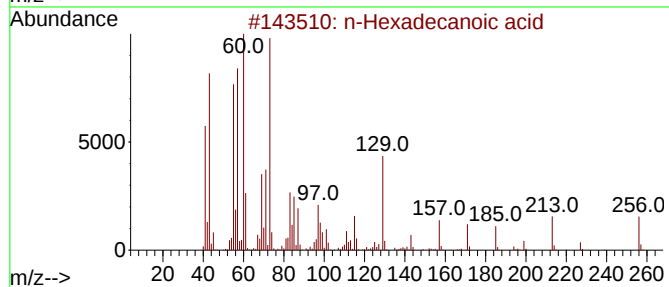
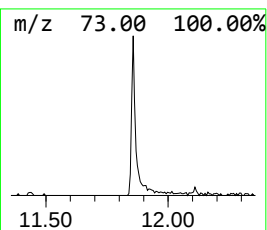
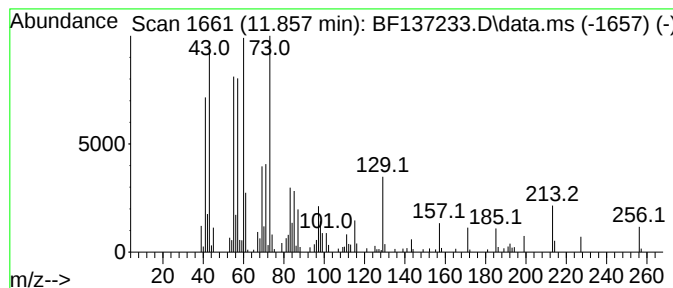
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	8.94 ng	203989	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	74



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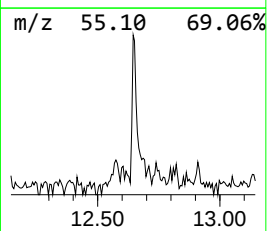
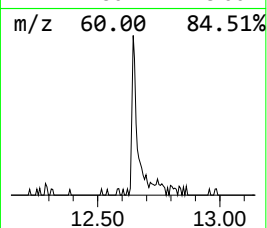
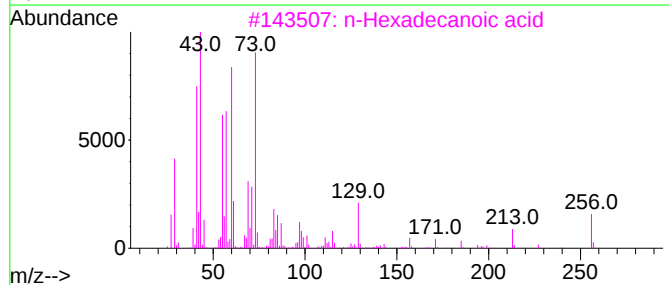
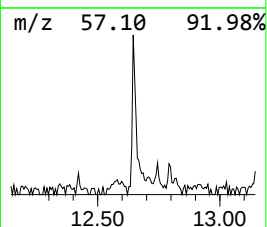
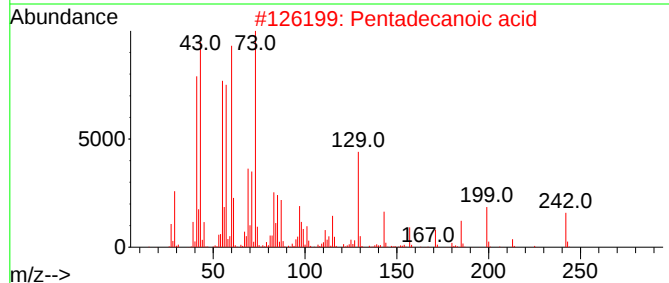
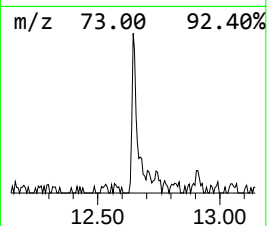
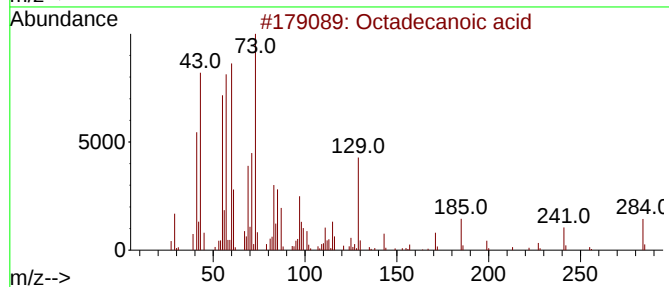
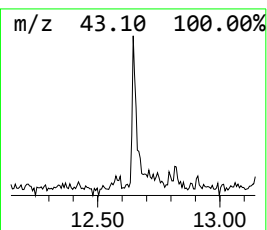
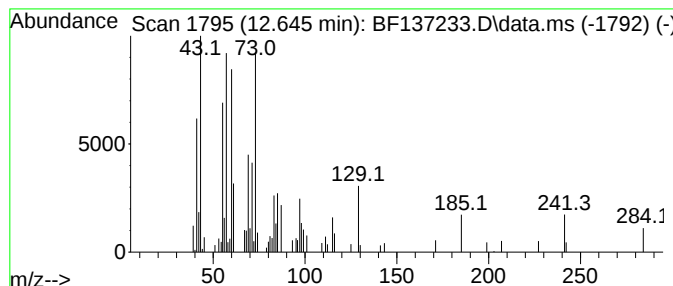
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	3.01 ng	74433	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4			Lactose	342	C12H22O11	000063-42-3	50
5			.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	25



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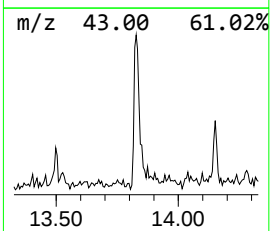
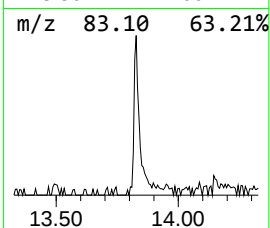
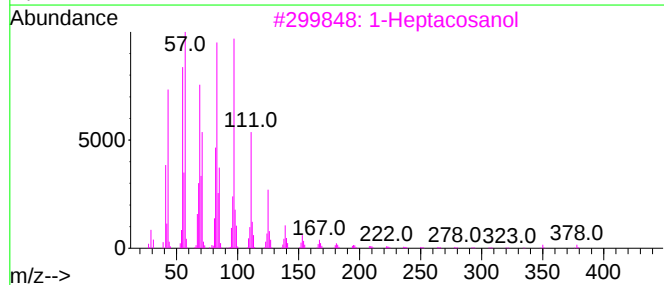
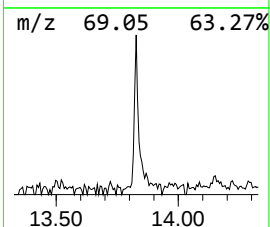
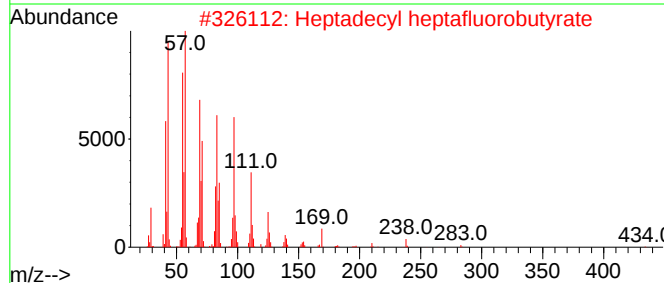
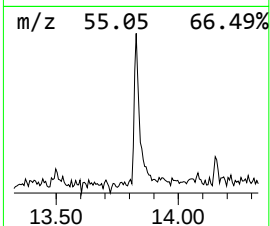
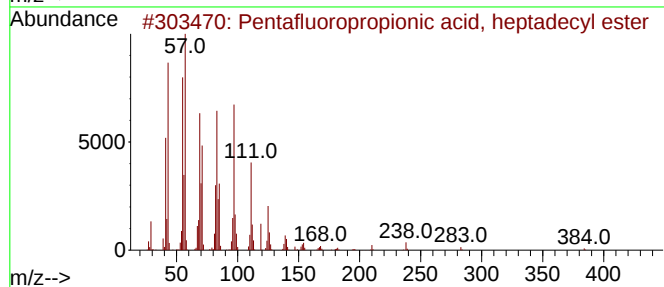
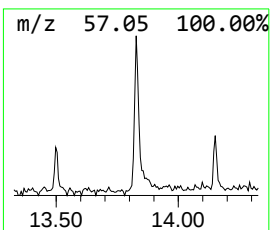
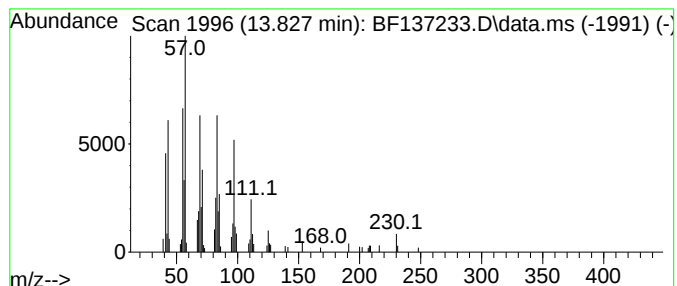
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	4.12 ng	101797	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			1-Hexacosanol	382	C26H54O	000506-52-5	91
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91



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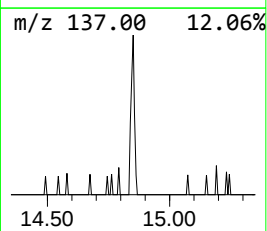
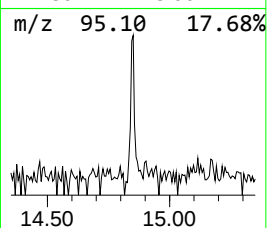
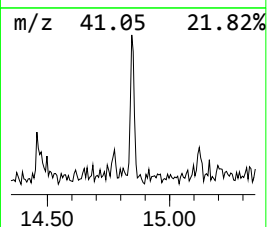
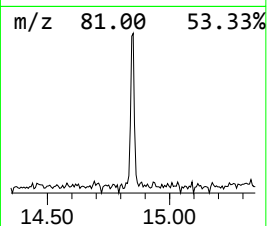
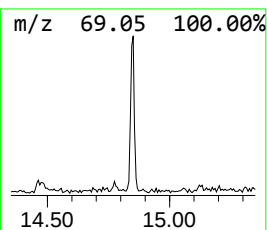
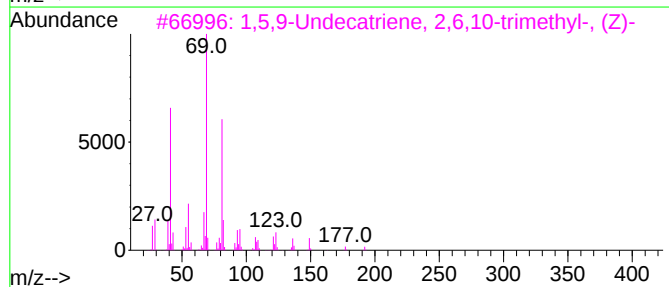
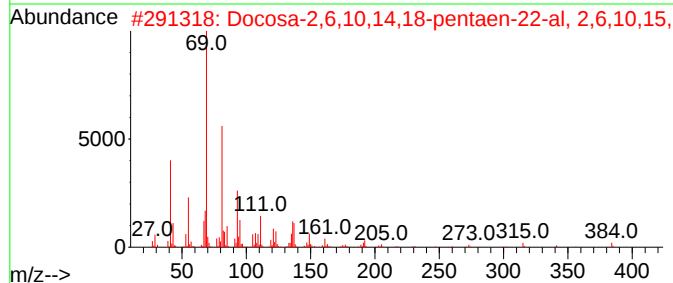
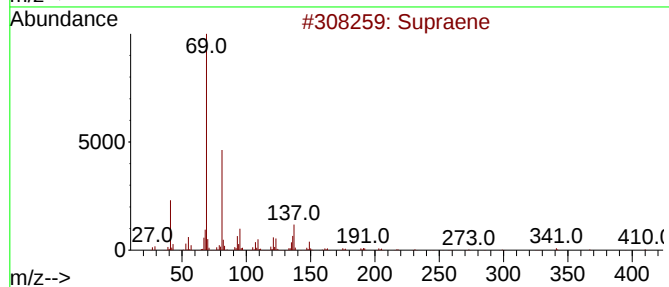
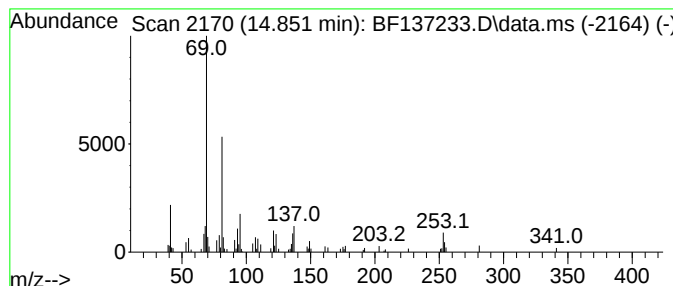
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Peak Number 5 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	3.00 ng	58413	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	74
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64
3			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
4			3,7,11-Tridecatricienoic acid, 4,8...	264	C17H28O2	036237-69-1	59
5			trans-Farnesol	222	C15H26O	000106-28-5	53



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ClientSampleId :
TR-614-COMP-01

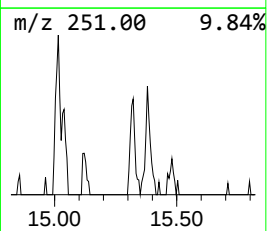
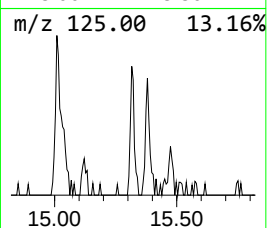
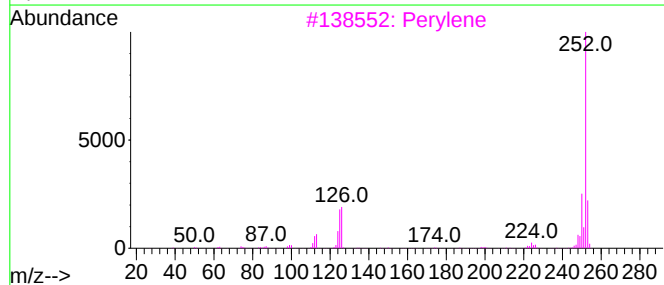
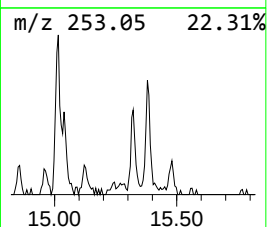
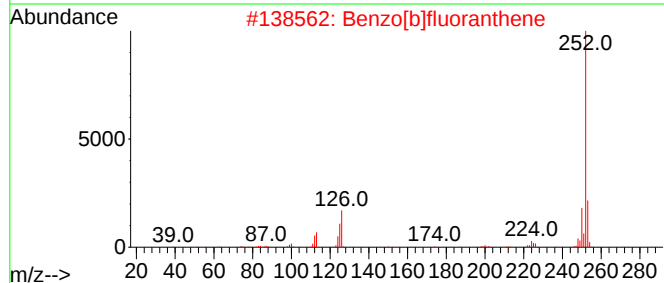
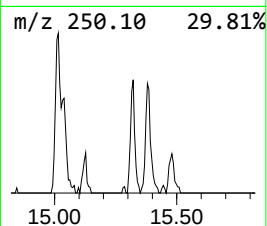
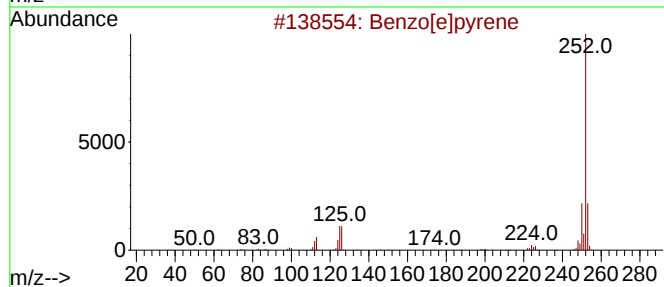
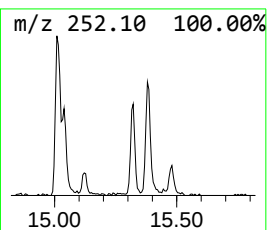
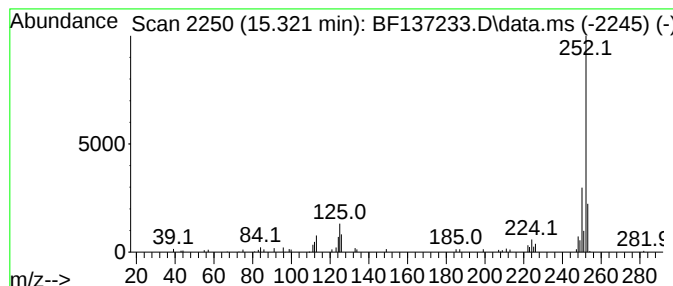
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.321	2.28 ng	44336	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	91
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	91
3			Perylene	252	C20H12	000198-55-0	90
4			Benzo[a]pyrene	252	C20H12	000050-32-8	87
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020124\
Data File : BF137233.D
Acq On : 01 Feb 2024 15:52
Operator : CG\JU
Sample : P1307-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-614-COMP-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.028	2.1	ng	38453	1	6.792	365420	20.0
n-Hexadecanoic ...	11.857	8.9	ng	203989	4	11.316	456232	20.0
Octadecanoic acid	12.645	3.0	ng	74433	5	13.968	494289	20.0
Pentafluoroprop...	13.827	4.1	ng	101797	5	13.968	494289	20.0
Supraene	14.851	3.0	ng	58413	6	15.445	389085	20.0
Benzo[e]pyrene	15.321	2.3	ng	44336	6	15.445	389085	20.0