

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
 Data File : BF136697.D
 Acq On : 22 Dec 2023 21:18
 Operator : CG\JU
 Sample : 05812-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RW2

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136697.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.857	123	131	135	rBV2	8833	16056	1.60%	0.255%
2	3.634	259	263	269	rBV2	9258	12885	1.29%	0.205%
3	3.851	296	300	306	rVB	9891	12859	1.29%	0.204%
4	4.998	493	495	500	rVB	24785	22815	2.28%	0.363%
5	5.092	507	511	515	rBV	76404	71467	7.14%	1.136%
6	5.422	563	567	577	rBV	108904	103404	10.34%	1.643%
7	6.428	735	738	744	rBV	77258	82071	8.20%	1.304%
8	6.610	766	769	780	rVB	24230	34337	3.43%	0.546%
9	6.781	795	798	801	rBV	527804	401991	40.18%	6.387%
10	6.845	806	809	813	rBV	15593	14018	1.40%	0.223%
11	7.339	889	893	896	rBV	685555	563634	56.34%	8.956%
12	7.598	934	937	940	rVB	52702	39630	3.96%	0.630%
13	8.057	1011	1015	1018	rBV	651098	501527	50.13%	7.969%
14	8.375	1066	1069	1086	rBV2	45992	87512	8.75%	1.391%
15	9.133	1194	1198	1201	rBV	1308586	1000378	100.00%	15.896%
16	9.216	1208	1212	1215	rBV	28403	21533	2.15%	0.342%
17	9.675	1283	1290	1295	rBV6	7989	17412	1.74%	0.277%
18	9.816	1310	1314	1317	rBV	569149	476108	47.59%	7.565%
19	9.916	1327	1331	1338	rBV	82532	113971	11.39%	1.811%
20	10.022	1345	1349	1354	rVB5	9943	13233	1.32%	0.210%
21	10.345	1399	1404	1408	rVB	18838	15544	1.55%	0.247%
22	10.604	1444	1448	1452	rBV	115480	95383	9.53%	1.516%
23	10.722	1465	1468	1474	rBV2	21797	28245	2.82%	0.449%
24	11.304	1563	1567	1570	rBV	479921	388216	38.81%	6.169%
25	11.604	1614	1618	1622	rBV2	13765	15276	1.53%	0.243%
26	11.704	1632	1635	1639	rVB2	16378	14961	1.50%	0.238%
27	11.845	1655	1659	1666	rBV	293967	309166	30.90%	4.913%
28	12.092	1698	1701	1705	rBV2	55531	45145	4.51%	0.717%
29	12.133	1705	1708	1712	rVB3	13881	16045	1.60%	0.255%
30	12.410	1751	1755	1759	rBV7	9573	18395	1.84%	0.292%
31	12.521	1771	1774	1776	rBV	19060	17342	1.73%	0.276%
32	12.627	1789	1792	1800	rBV	75760	88956	8.89%	1.413%
33	12.751	1811	1813	1816	rVB	16180	12630	1.26%	0.201%
34	12.898	1834	1838	1844	rVB	585565	471845	47.17%	7.497%
35	13.810	1991	1993	1995	rBV3	20086	17228	1.72%	0.274%
36	13.845	1995	1999	2011	rVV3	86432	231311	23.12%	3.675%

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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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.957	2014	2018	2021	rBV	418025	377288	37.71%	5.995%
38	14.104	2040	2043	2045	rBV	45474	42995	4.30%	0.683%
39	14.821	2162	2165	2168	rVB	83832	84734	8.47%	1.346%
40	15.433	2265	2269	2274	rVB	313163	395861	39.57%	6.290%

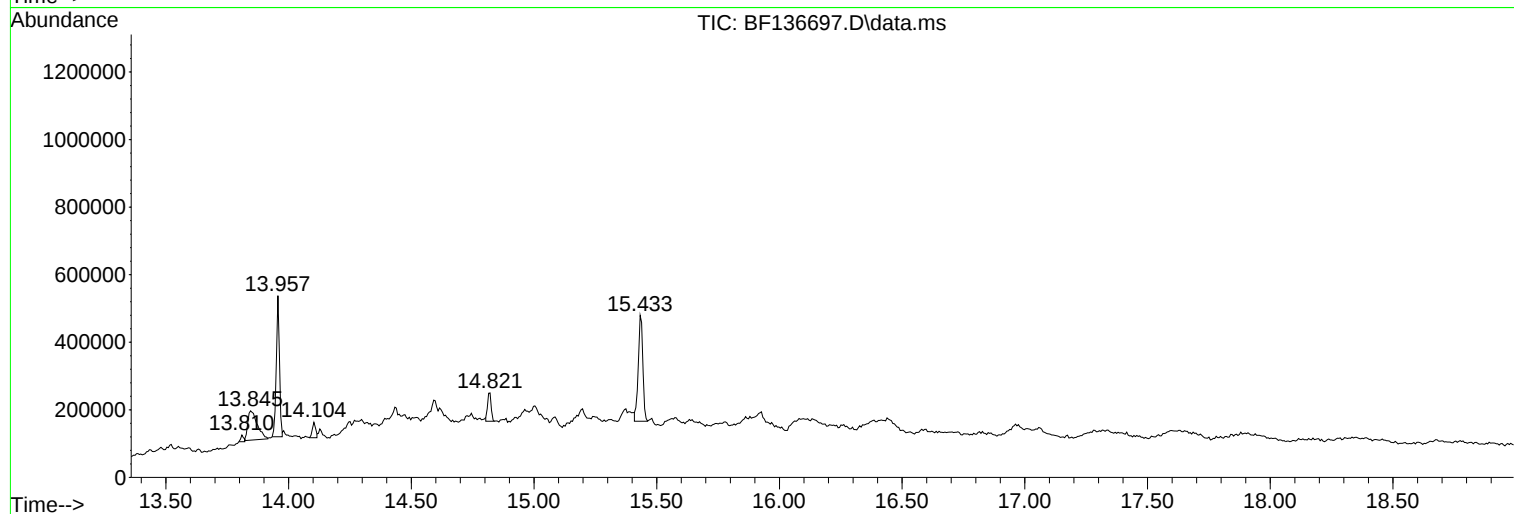
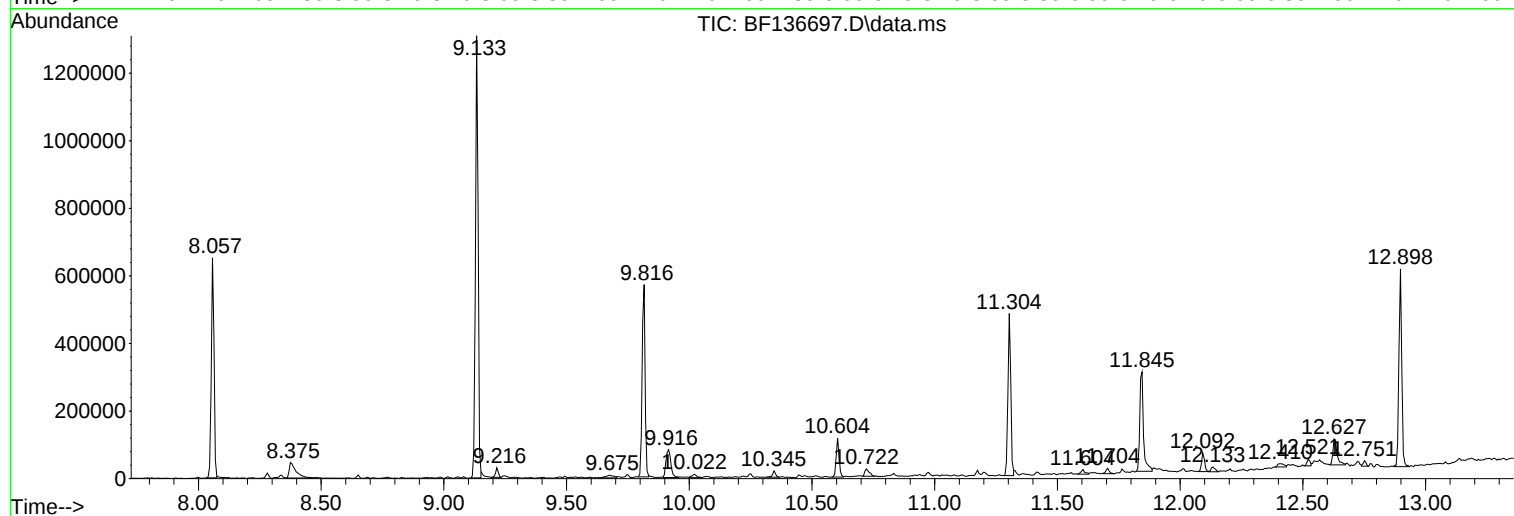
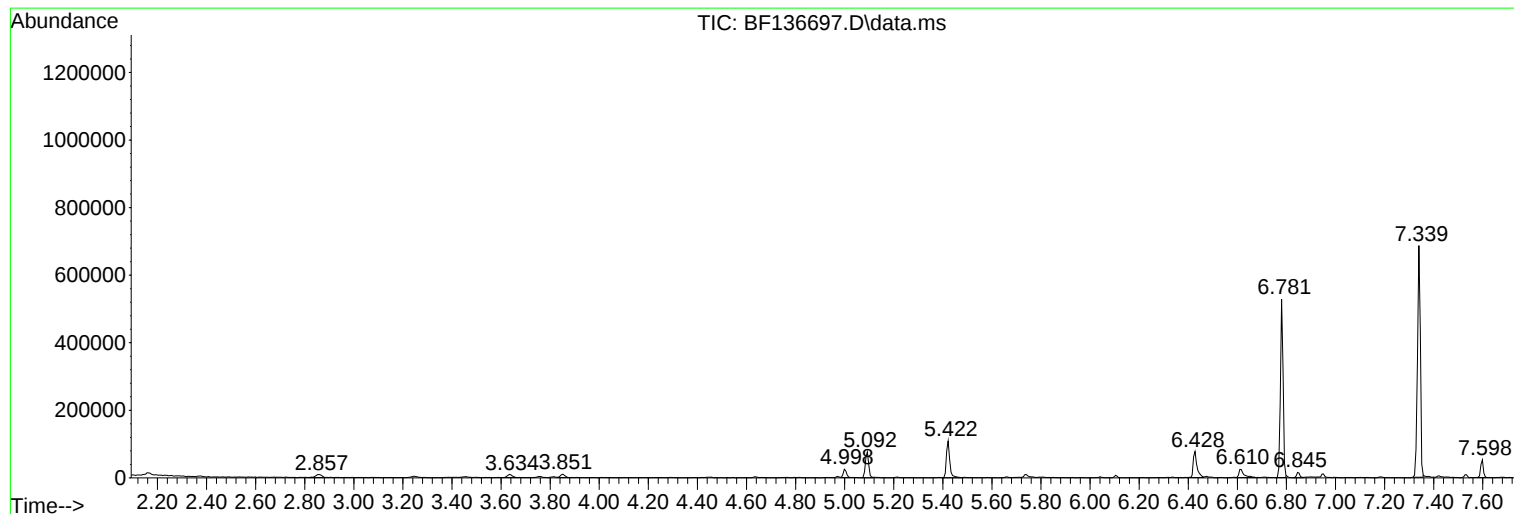
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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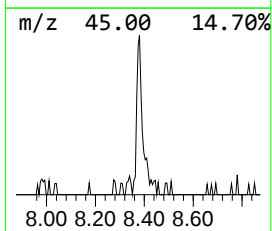
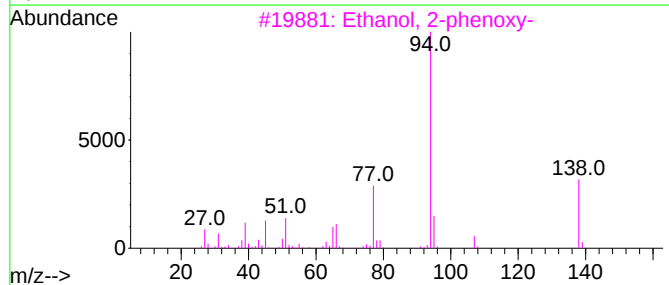
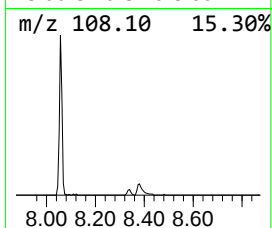
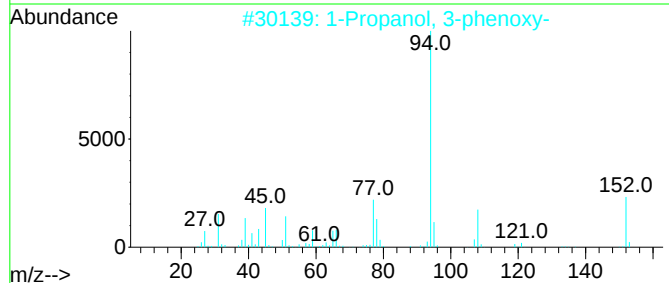
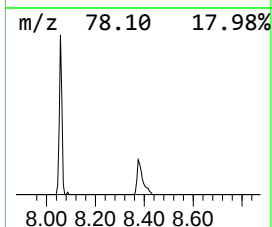
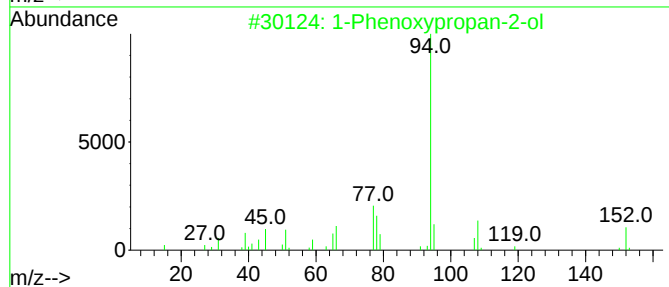
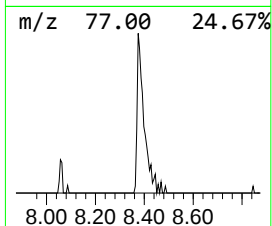
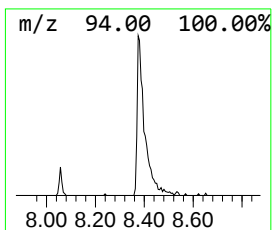
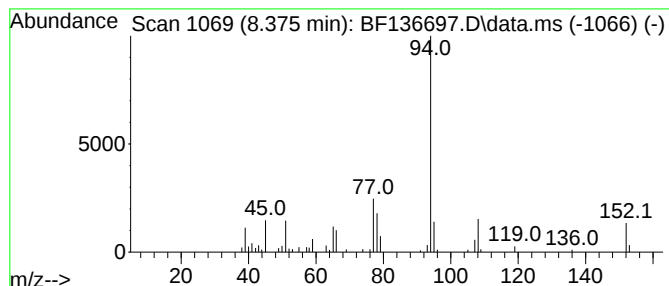
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.375	3.49 ng	87512	Naphthalene-d8	8.057

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	97
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
5		Benzene, (1-methylpropoxy)-	150	C10H14O	010574-17-1	53



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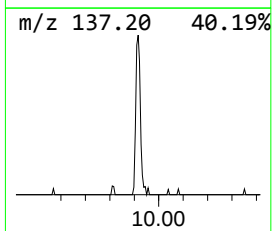
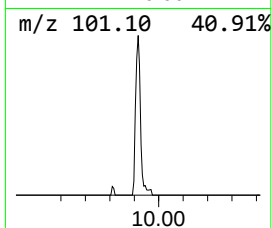
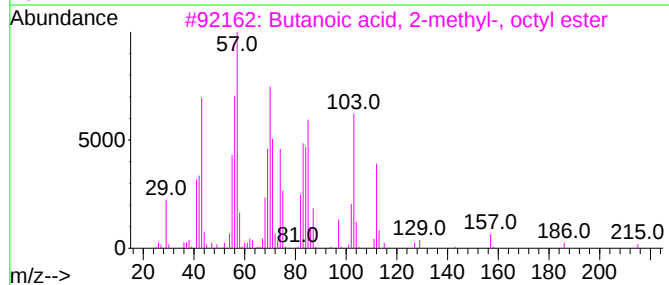
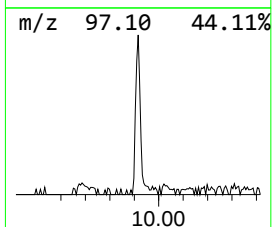
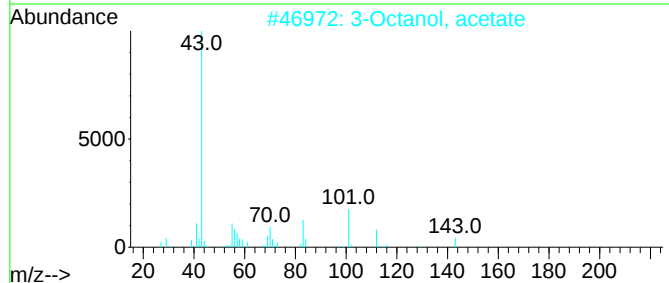
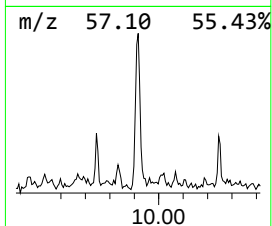
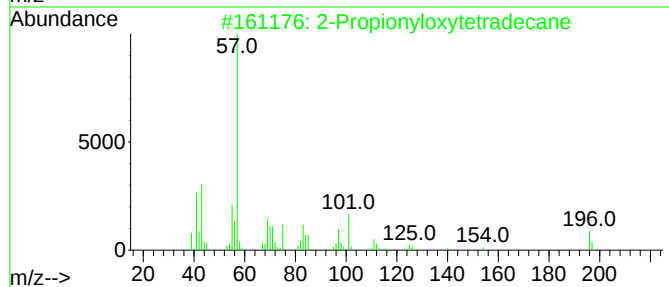
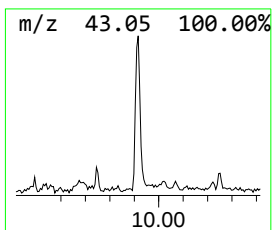
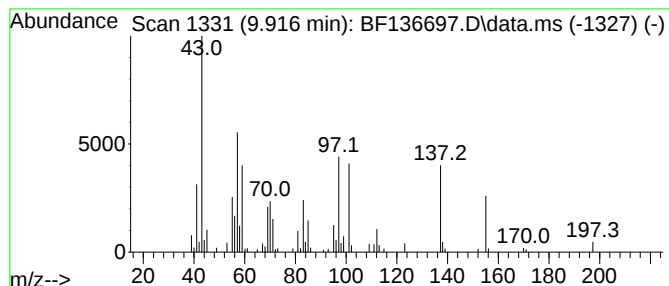
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown9.916 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.916	4.79 ng	113971	Acenaphthene-d10	9.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propionyloxytetradecane		270	C17H34O2	1000245-62-7	27	
2	3-Octanol, acetate		172	C10H20O2	004864-61-3	22	
3	Butanoic acid, 2-methyl-, octyl ...		214	C13H26O2	029811-50-5	10	
4	7-Oxabicyclo[4.1.0]heptane, 1-me...		112	C7H12O	001713-33-3	10	
5	2,4,4-Trimethyl-1-pentanol, chlo...		242	C10H17ClF2O2	1000447-27-2	10	



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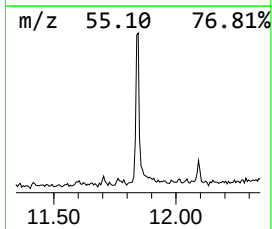
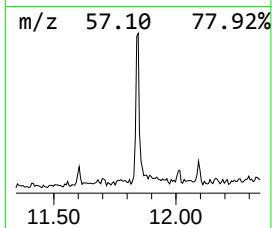
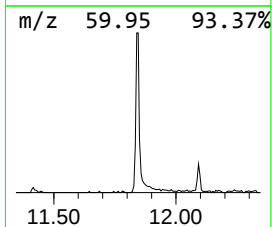
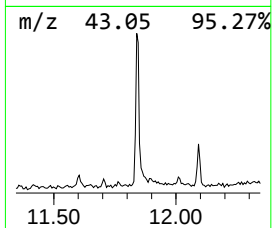
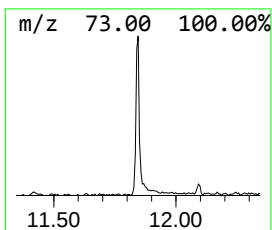
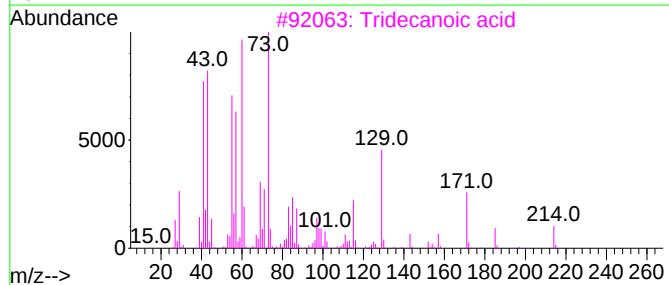
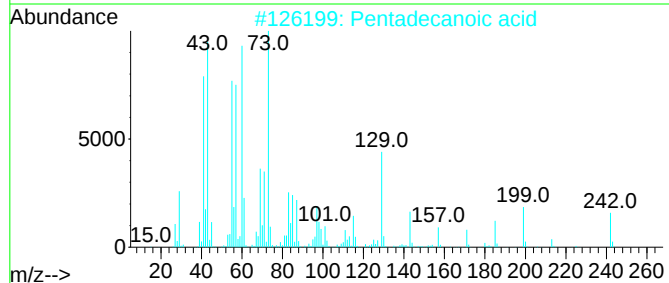
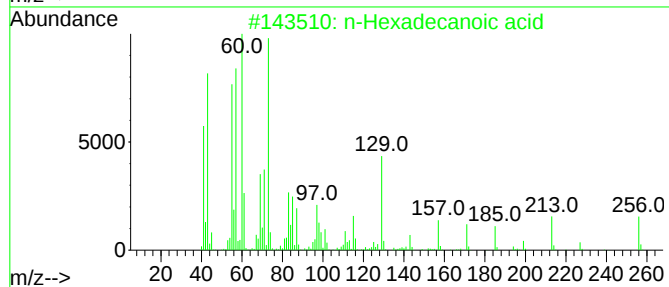
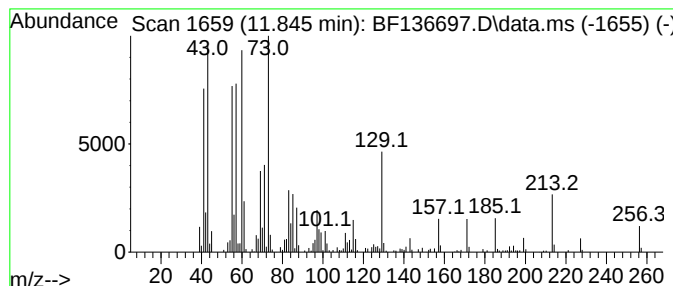
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	15.93 ng	309166	Phenanthrene-d10	11.304

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	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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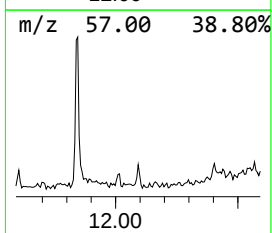
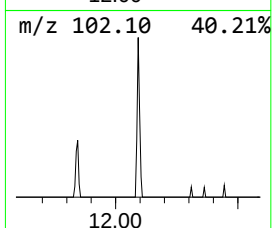
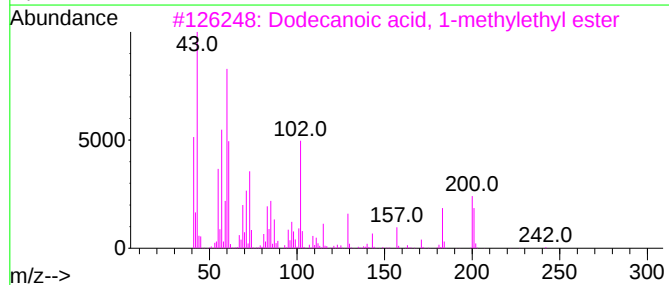
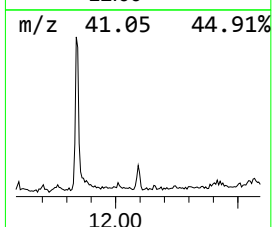
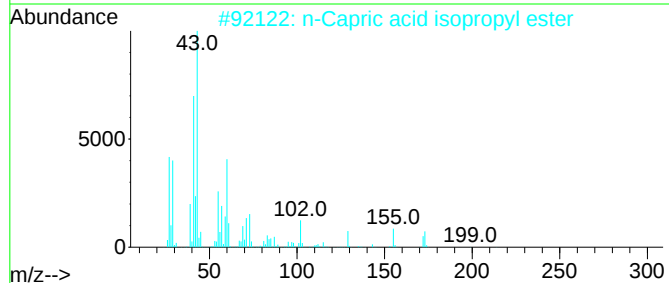
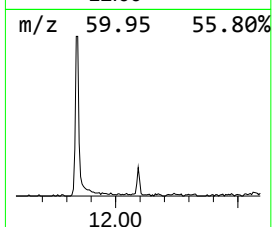
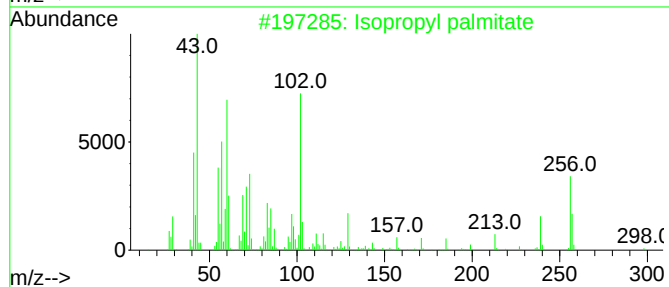
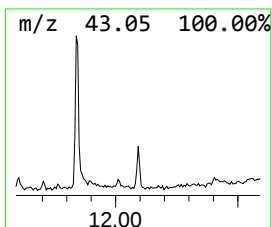
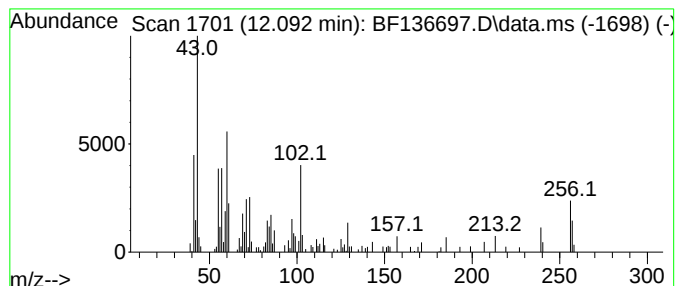
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Isopropyl palmitate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.092	2.33 ng	45145	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	91
2			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	43
3			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	43
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	38
5			.alpha.-Methyl-D-mannopyranoside	194	C7H14O6	000617-04-9	35



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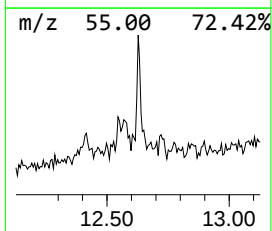
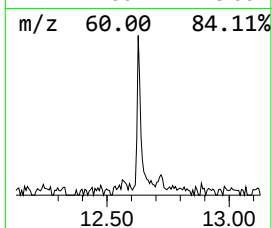
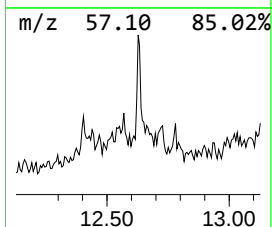
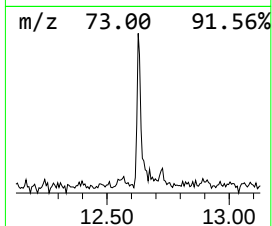
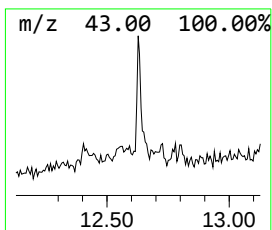
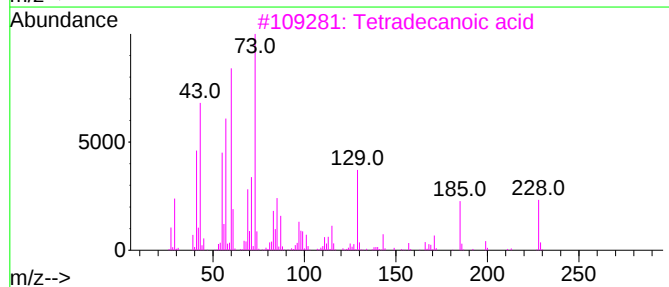
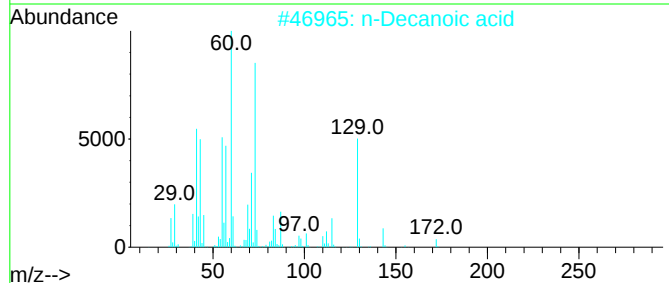
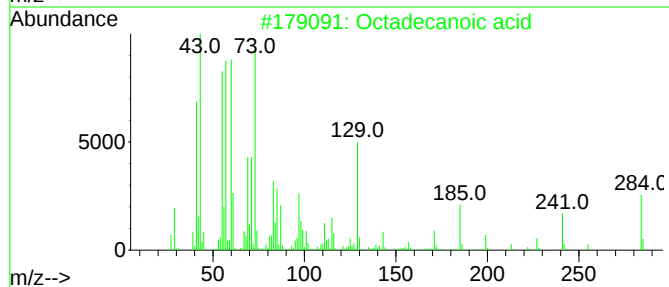
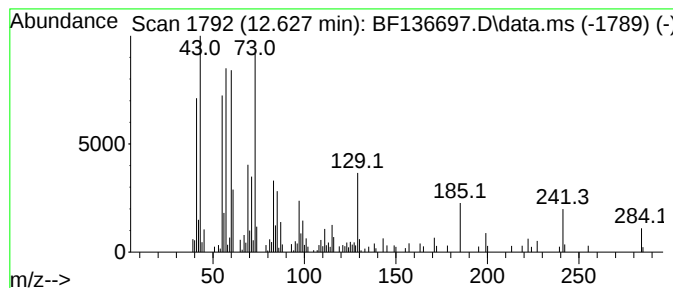
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	4.58 ng	88956	Phenanthrene-d10	11.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			n-Decanoic acid	172	C10H20O2	000334-48-5	70
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5			Tridecanoic acid	214	C13H26O2	000638-53-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136697.D
Acq On : 22 Dec 2023 21:18
Operator : CG\JU
Sample : 05812-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

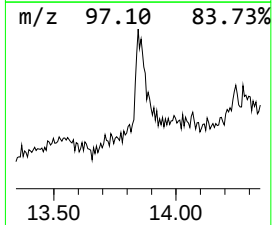
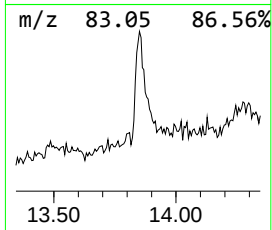
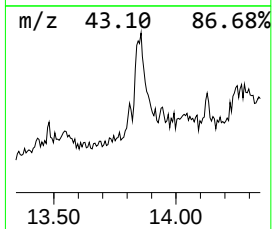
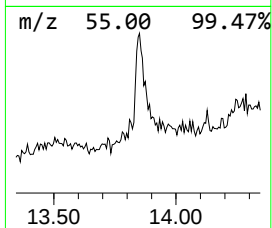
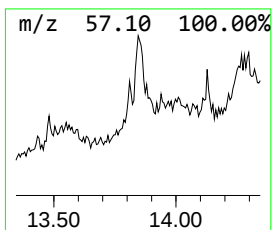
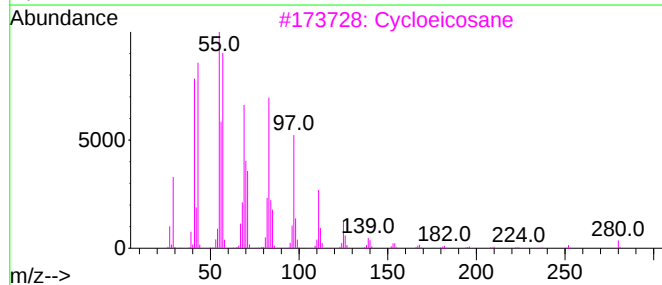
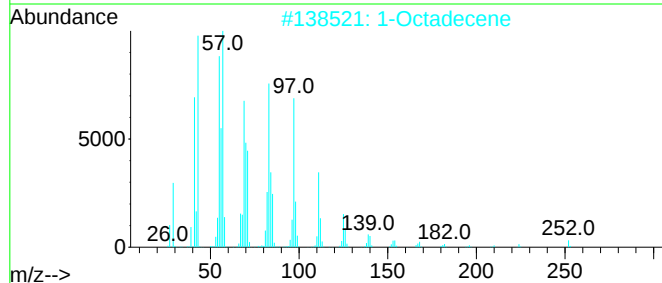
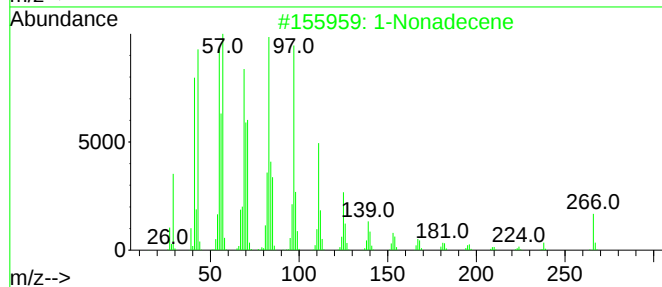
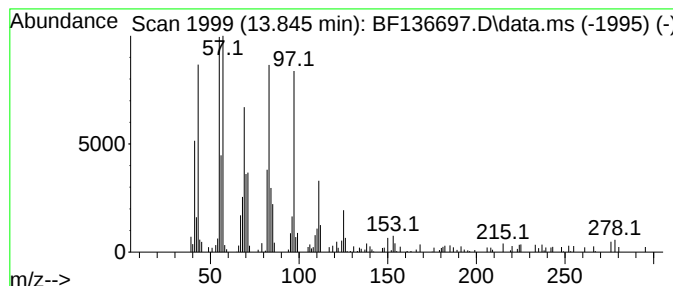
Instrument :
BNA_F
ClientSampleId :
RW2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Nonadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.845	12.26 ng	231311	Chrysene-d12	13.957	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	94
2	1-Octadecene	252	C18H36	000112-88-9	93
3	Cycloeicosane	280	C20H40	000296-56-0	93
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136697.D
Acq On : 22 Dec 2023 21:18
Operator : CG\JU
Sample : 05812-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW2

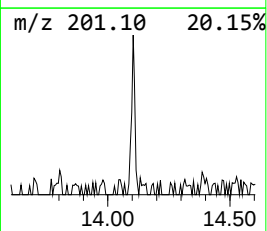
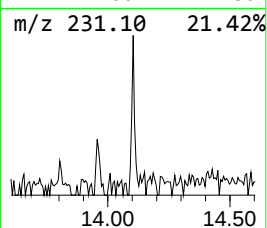
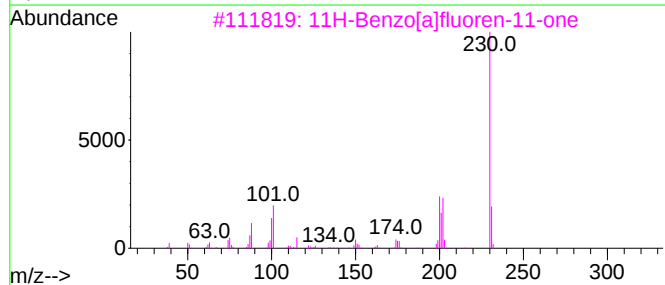
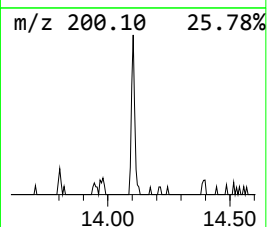
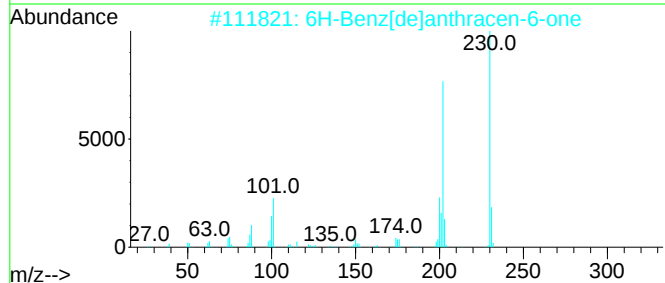
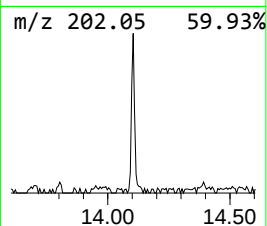
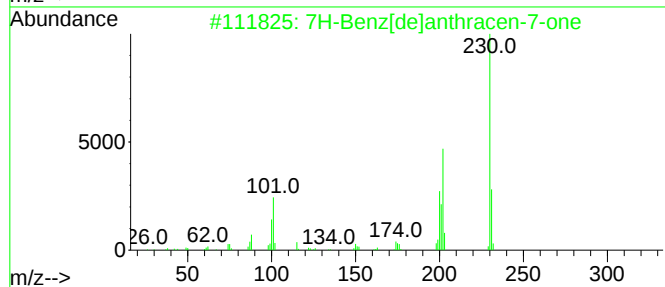
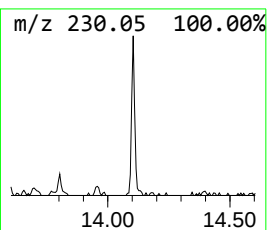
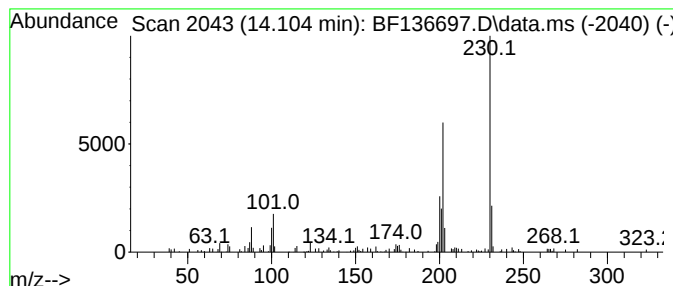
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 7H-Benz[de]anthracen-7-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.104	2.28 ng	42995	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	97
2			6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	93
3			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	89
4			4-Pyrenecarbaldehyde	230	C17H10O	022245-51-8	58
5			1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136697.D
Acq On : 22 Dec 2023 21:18
Operator : CG\JU
Sample : 05812-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

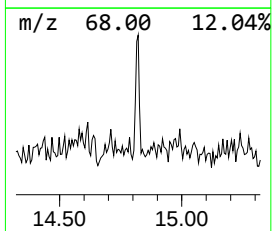
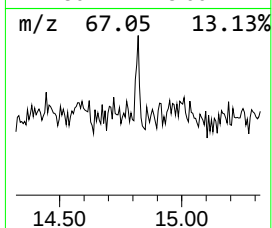
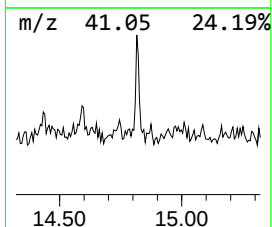
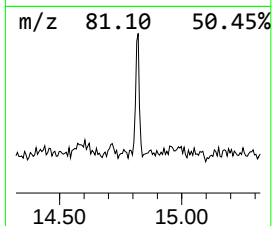
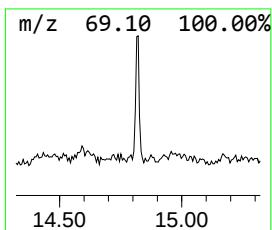
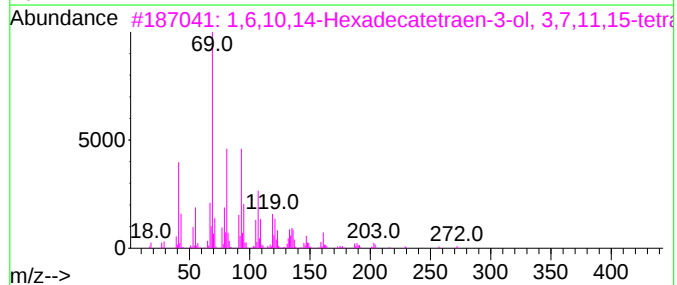
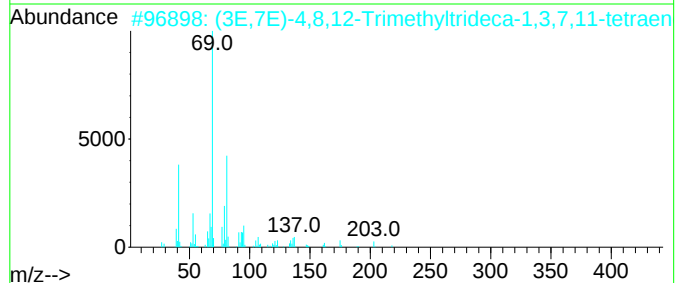
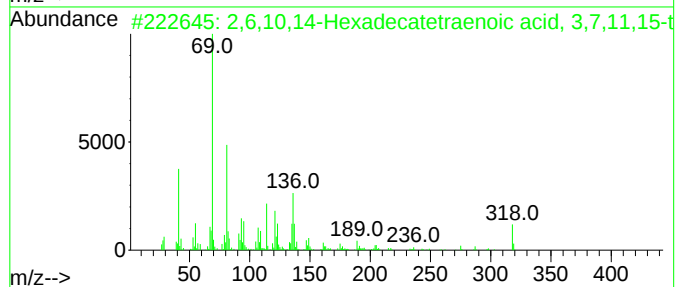
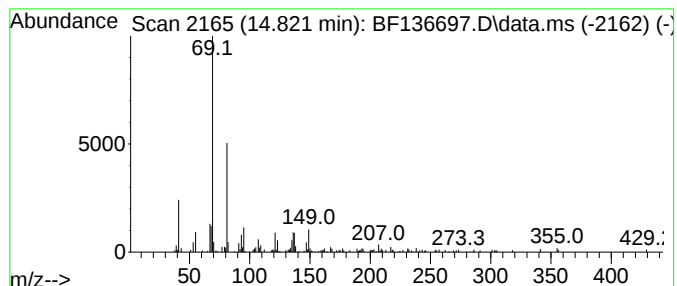
Instrument :
BNA_F
ClientSampleId :
RW2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,6,10,14-Hexadecatetraenoic... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.821	4.28 ng	84734	Perylene-d12	15.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	64
2	(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	58
3	1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	53
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	53
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
Data File : BF136697.D
Acq On : 22 Dec 2023 21:18
Operator : CG\JU
Sample : 05812-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
1-Phenoxypropan...	8.375	3.5	ng	87512	2	8.057	501527	20.0
unknown9.916	9.916	4.8	ng	113971	3	9.816	476108	20.0
n-Hexadecanoic ...	11.845	15.9	ng	309166	4	11.304	388216	20.0
Isopropyl palmi...	12.092	2.3	ng	45145	4	11.304	388216	20.0
Octadecanoic acid	12.627	4.6	ng	88956	4	11.304	388216	20.0
1-Nonadecene	13.845	12.3	ng	231311	5	13.957	377288	20.0
7H-Benz[de]anth...	14.104	2.3	ng	42995	5	13.957	377288	20.0
2,6,10,14-Hexad...	14.821	4.3	ng	84734	6	15.433	395861	20.0