

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
 Data File : BF136857.D
 Acq On : 30 Dec 2023 06:48
 Operator : CG\JU
 Sample : 05897-12
 Misc :
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-41

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: BF136857.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.875	127	134	144	rVB	16610	25629	1.49%	0.223%
2	3.322	207	210	225	rBV	50667	102832	5.99%	0.894%
3	5.016	494	498	503	rBV	32449	35322	2.06%	0.307%
4	5.422	563	567	583	rBV	1487204	1323598	77.14%	11.503%
5	6.428	733	738	751	rBV	1484997	1418562	82.67%	12.329%
6	6.616	767	770	782	rBV	18207	28855	1.68%	0.251%
7	6.781	794	798	801	rBV	525781	420167	24.49%	3.652%
8	7.339	888	893	896	rBV	934727	921612	53.71%	8.010%
9	8.057	1011	1015	1018	rBV	686820	546926	31.87%	4.753%
10	8.375	1066	1069	1080	rBV	35729	50844	2.96%	0.442%
11	9.133	1194	1198	1201	rBV	2088123	1715949	100.00%	14.913%
12	9.810	1310	1313	1326	rBV	663059	615614	35.88%	5.350%
13	9.916	1326	1331	1344	rVB	141163	197214	11.49%	1.714%
14	10.604	1445	1448	1460	rBV	618495	539982	31.47%	4.693%
15	11.304	1563	1567	1571	rBV	761842	617424	35.98%	5.366%
16	11.704	1632	1635	1640	rVB2	37182	29721	1.73%	0.258%
17	12.416	1749	1756	1762	rBV4	23554	33103	1.93%	0.288%
18	12.904	1834	1839	1842	rBV	1729430	1451265	84.58%	12.613%
19	13.133	1876	1878	1881	rVB	27653	20869	1.22%	0.181%
20	13.757	1976	1984	1990	rBV5	22068	35899	2.09%	0.312%
21	13.863	1995	2002	2003	rBV4	15245	23960	1.40%	0.208%
22	13.963	2015	2019	2029	rVB	392234	397316	23.15%	3.453%
23	14.251	2064	2068	2072	rVB2	20191	22050	1.29%	0.192%
24	14.433	2093	2099	2103	rBV	23377	25781	1.50%	0.224%
25	15.086	2205	2210	2216	rBV2	59035	67489	3.93%	0.587%
26	15.439	2265	2270	2283	rVB	285031	409665	23.87%	3.560%
27	15.680	2307	2311	2317	rBV4	17500	25023	1.46%	0.217%
28	15.921	2347	2352	2357	rBV	59536	86942	5.07%	0.756%
29	16.062	2369	2376	2380	rBV6	9292	23328	1.36%	0.203%
30	16.745	2486	2492	2499	rVB4	27038	49603	2.89%	0.431%
31	17.062	2540	2546	2547	rBV3	17726	28390	1.65%	0.247%
32	17.098	2547	2552	2559	rVB3	60159	120932	7.05%	1.051%
33	18.245	2740	2747	2760	rVB9	18589	70188	4.09%	0.610%
34	18.592	2798	2806	2807	rBV6	14351	24248	1.41%	0.211%

Sum of corrected areas: 11506302

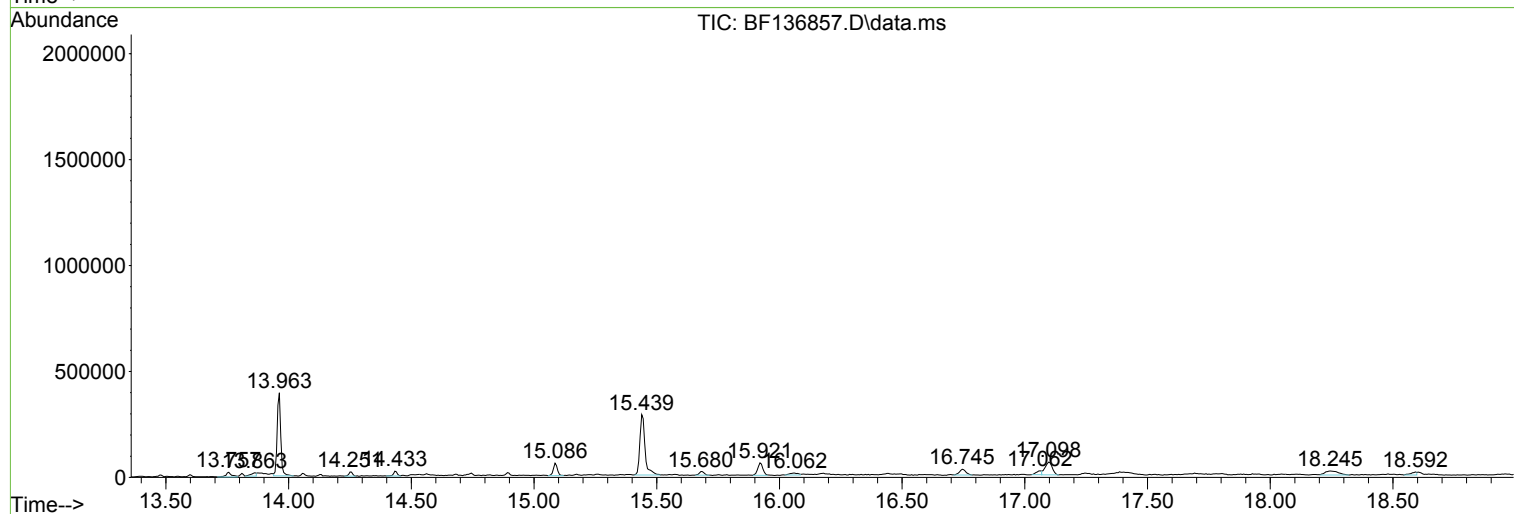
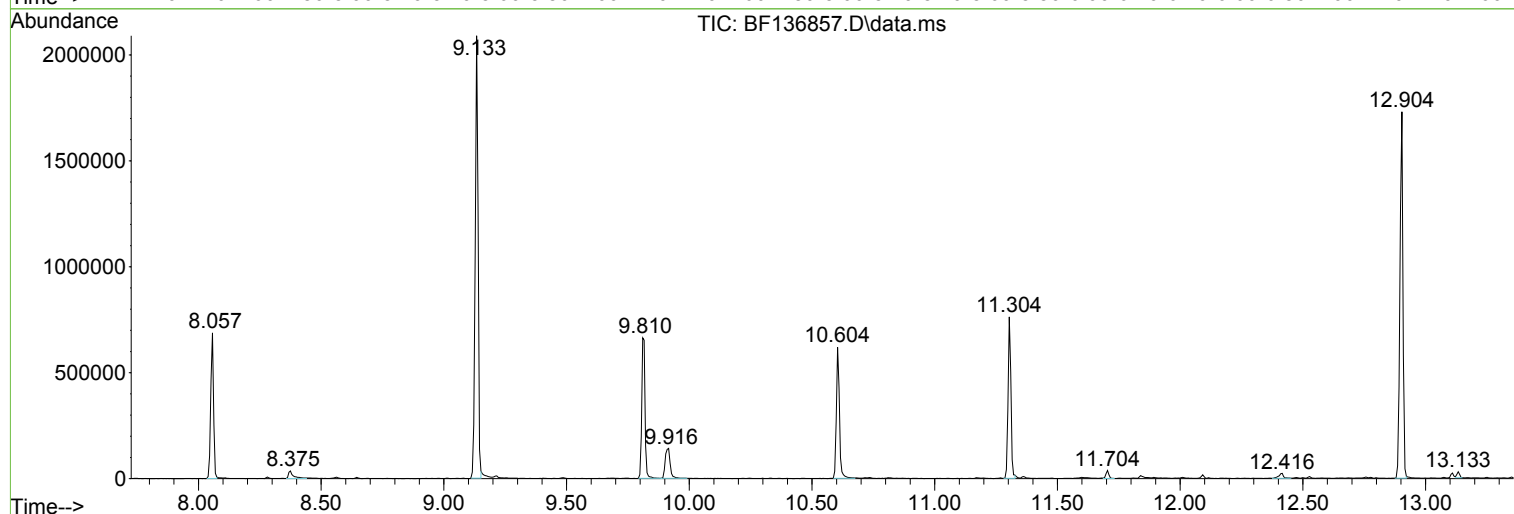
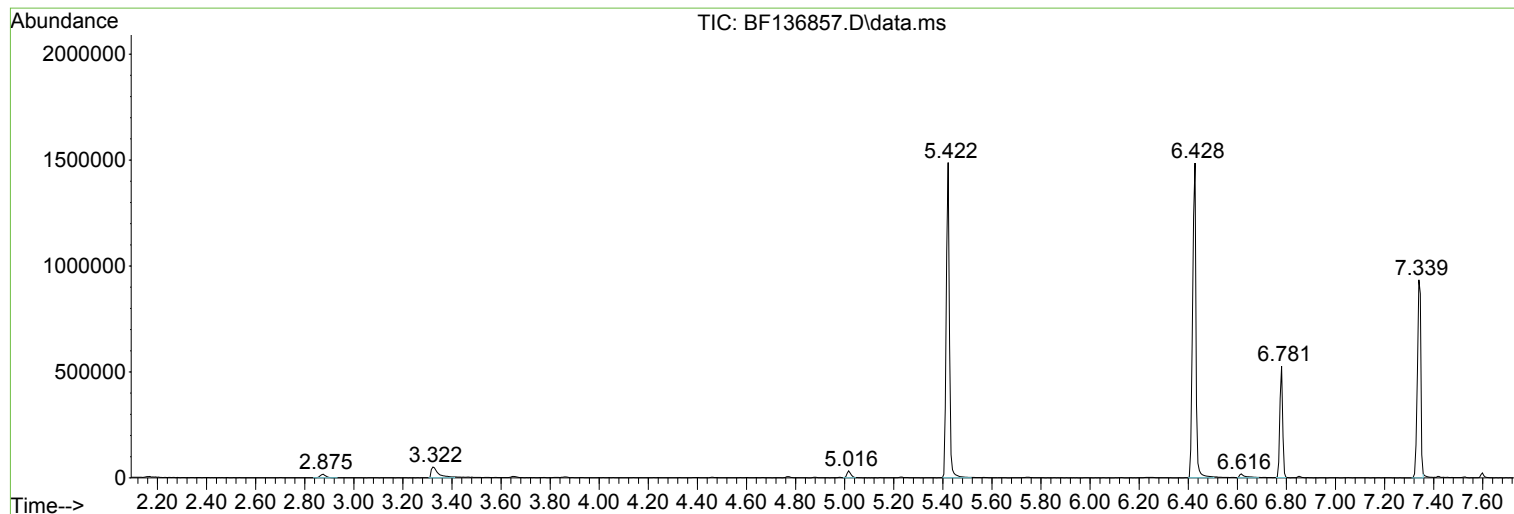
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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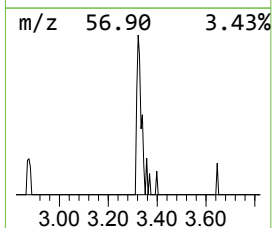
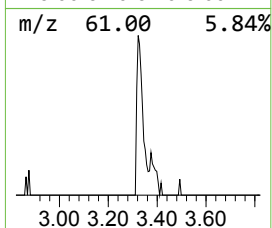
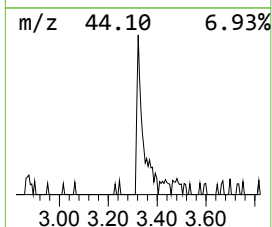
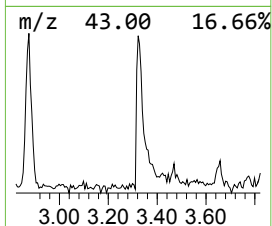
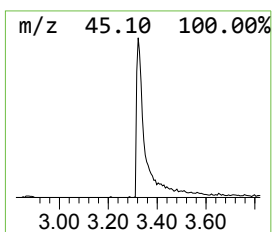
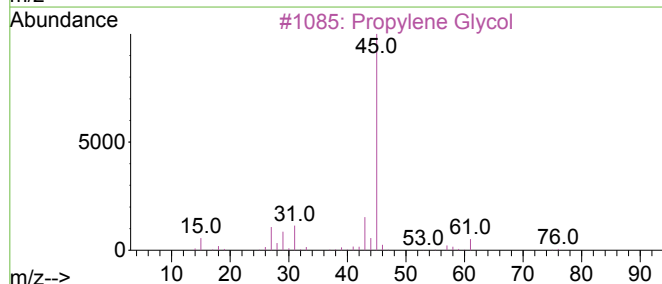
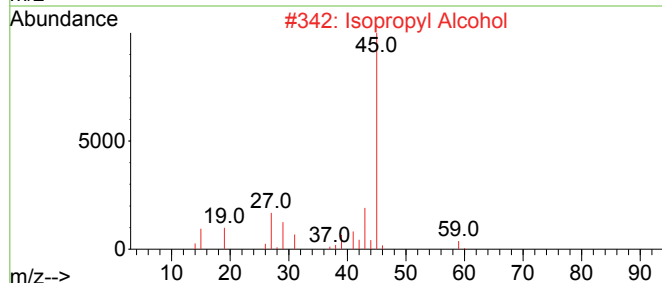
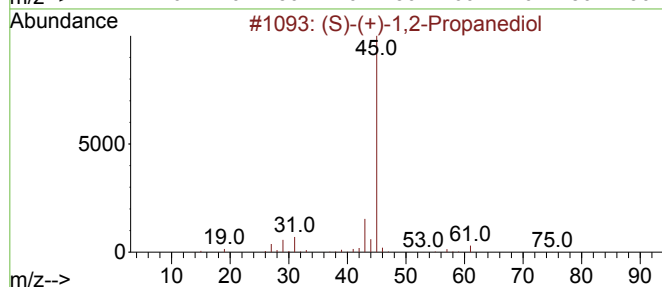
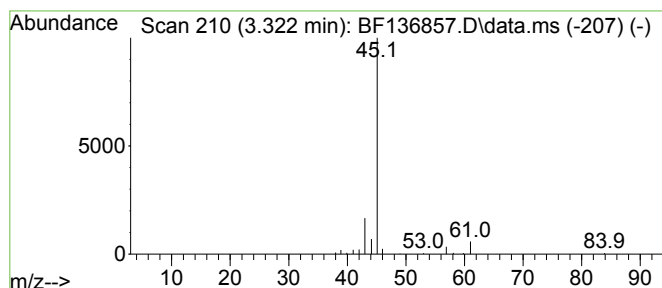
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.322 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.322	4.89 ng	102832	1,4-Dichlorobenzene-d4	6.781

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol		76	C3H8O2	004254-15-3	43
2	Isopropyl Alcohol		60	C3H8O	000067-63-0	9
3	Propylene Glycol		76	C3H8O2	000057-55-6	9
4	2-Butanol		74	C4H10O	000078-92-2	9
5	Butanenitrile, 2-(methoxymethoxy)		129	C6H11NO2	1000196-86-5	9



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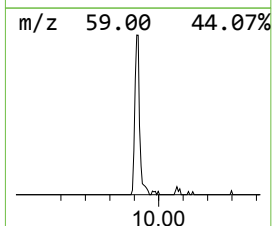
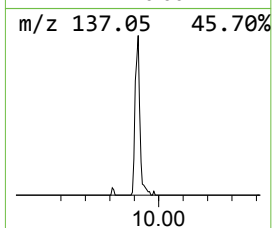
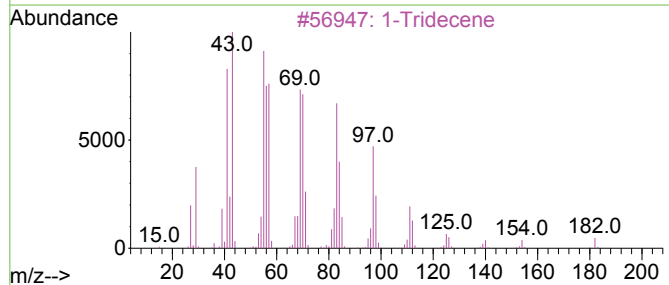
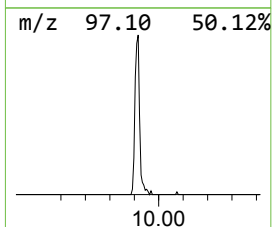
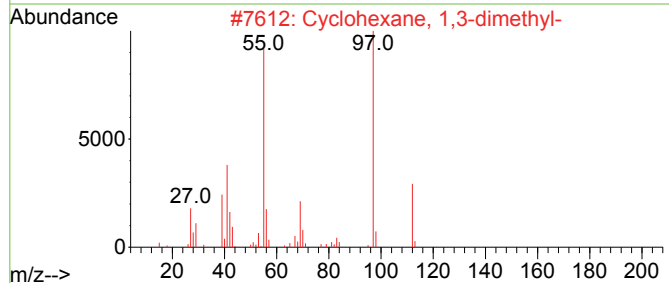
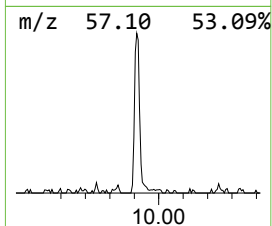
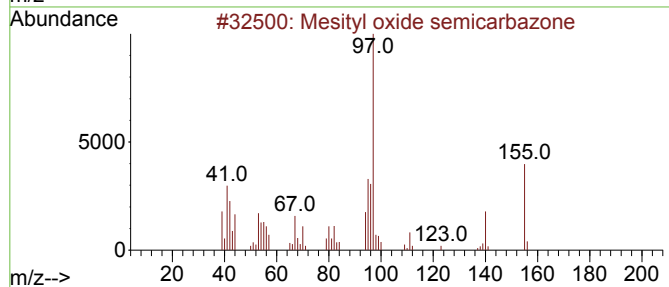
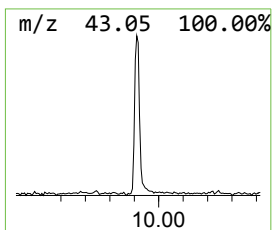
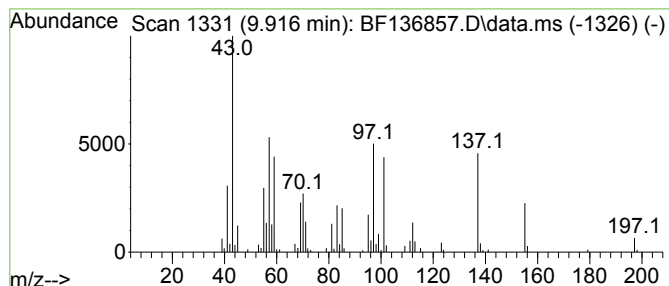
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown9.916 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.916	6.41 ng	197214	Acenaphthene-d10	9.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesityl oxide semicarbazone	155	C7H13N3O	003780-62-9	11
2			Cyclohexane, 1,3-dimethyl-	112	C8H16	000591-21-9	11
3			1-Tridecene	182	C13H26	002437-56-1	10
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
5			Succinic acid, 2-methylpent-3-yl...	298	C17H30O4	1000390-06-8	10



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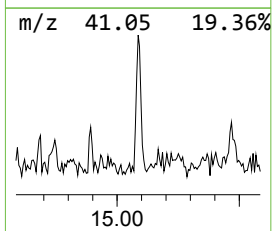
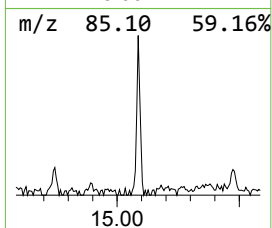
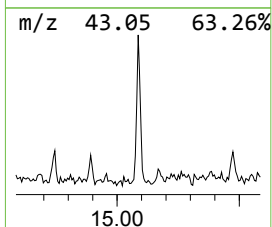
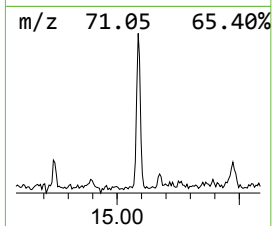
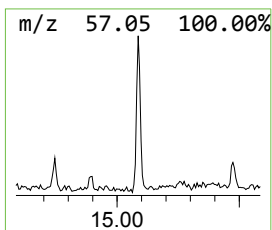
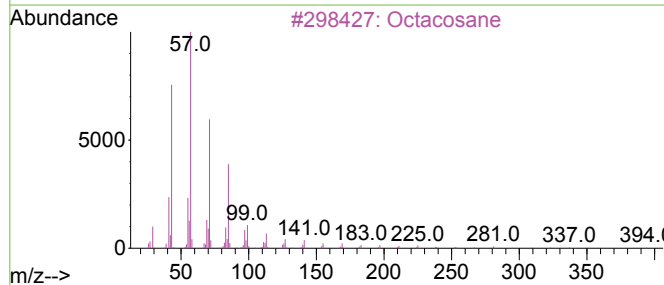
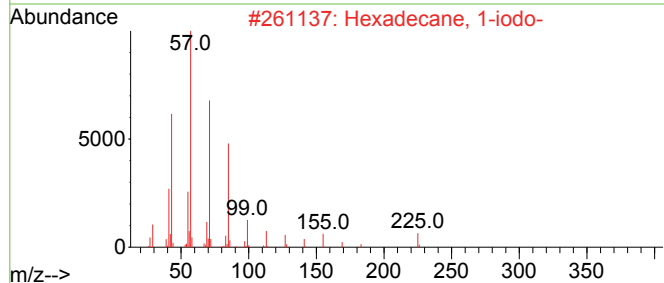
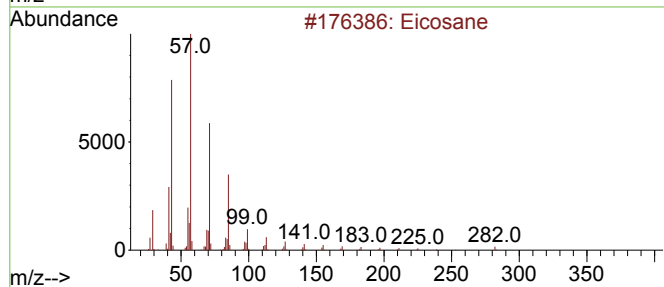
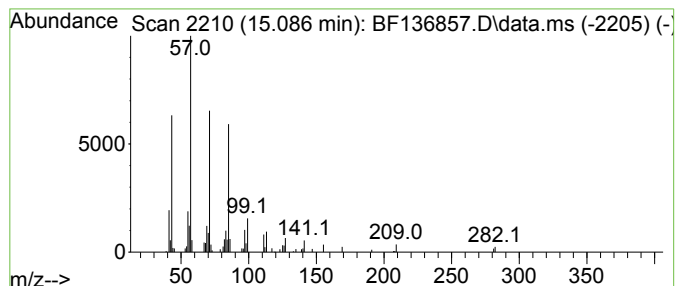
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	3.29 ng	67489	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
3			Octacosane	394	C28H58	000630-02-4	74
4			Heptacosane	380	C27H56	000593-49-7	74
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	72



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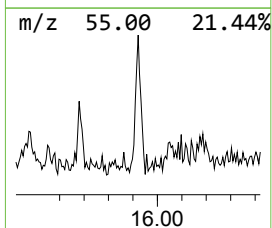
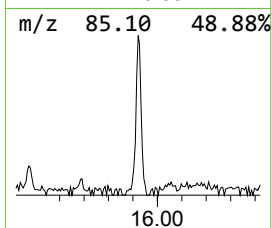
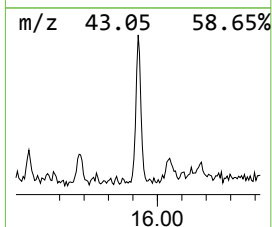
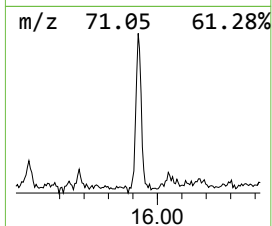
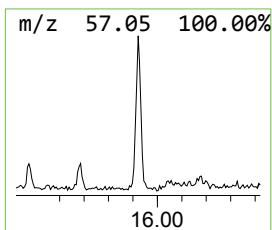
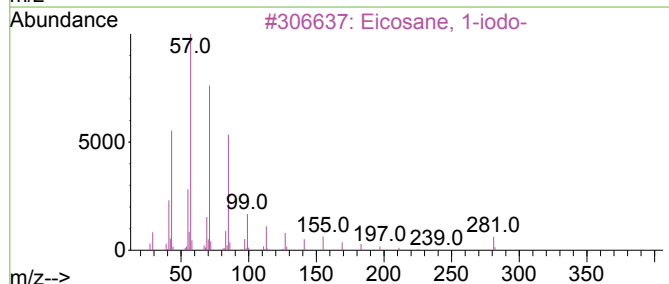
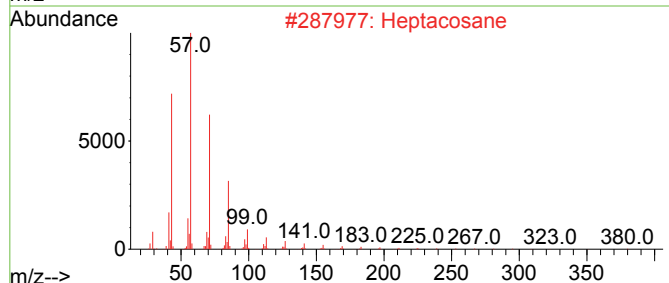
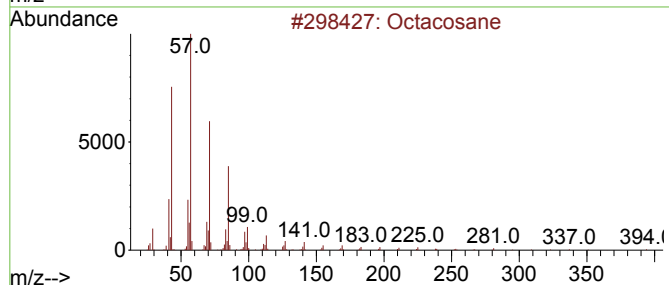
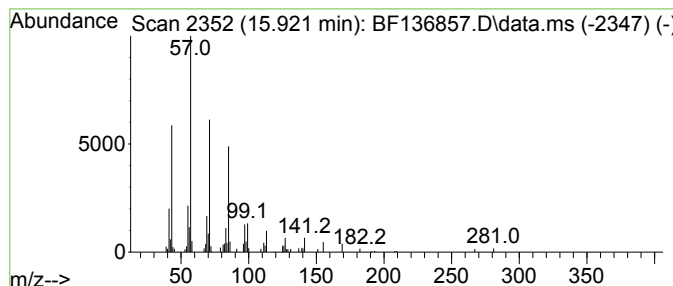
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	4.24 ng	86942	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Heptacosane	380	C27H56	000593-49-7	90
3			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	90
4			Triacontane	422	C30H62	000638-68-6	90
5			Pentacosane	352	C25H52	000629-99-2	87



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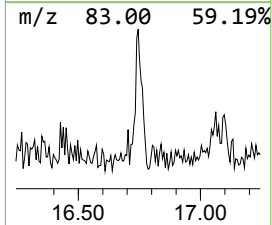
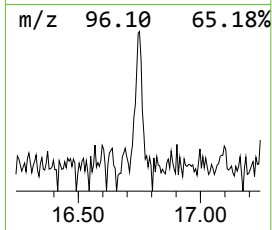
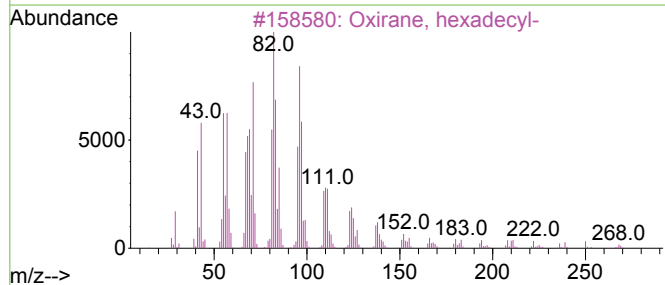
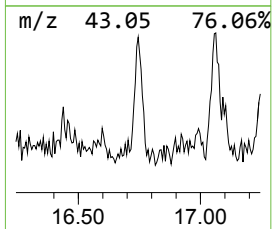
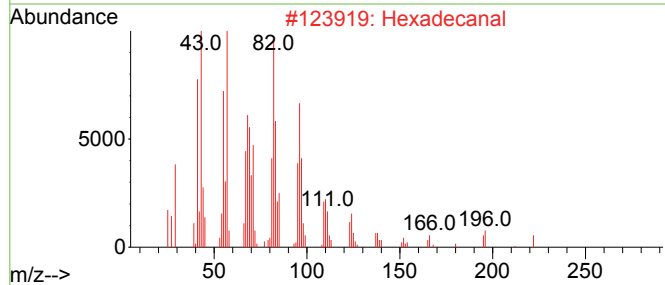
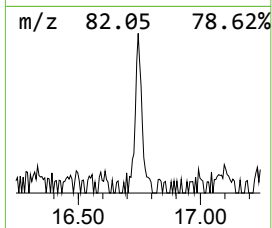
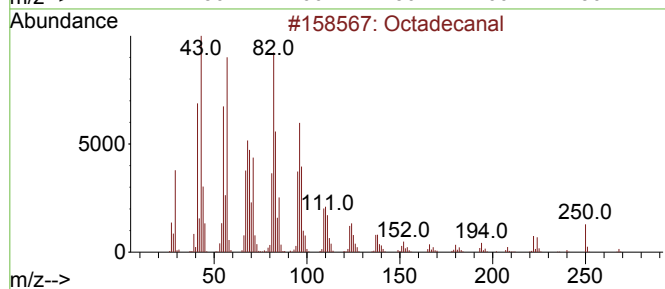
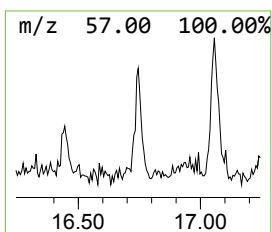
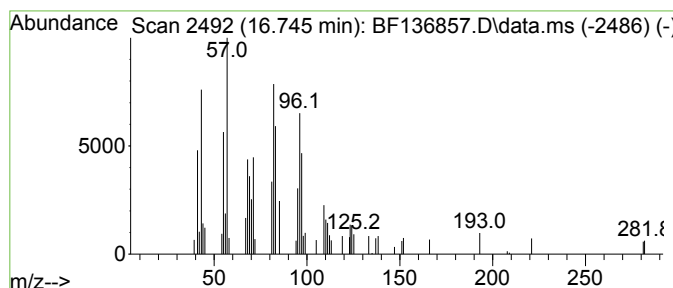
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Peak Number 5 Octadecanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.745	2.42 ng	49603	Perylene-d12	15.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	90
2			Hexadecanal	240	C16H32O	000629-80-1	90
3			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
4			Eicosanal-	296	C20H40O	002400-66-0	87
5			Tetradecanal	212	C14H28O	000124-25-4	72



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ALS Vial : 39 Sample Multiplier: 1

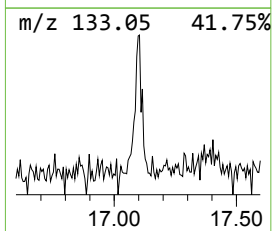
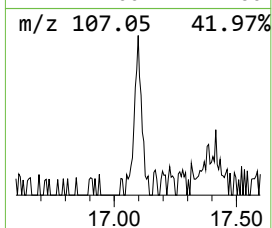
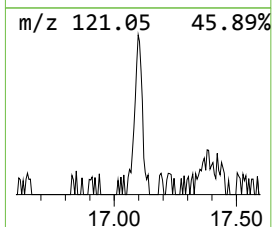
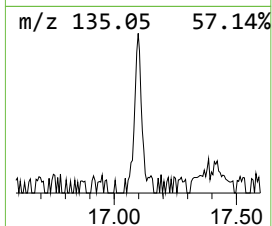
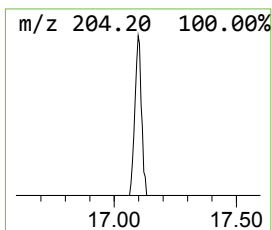
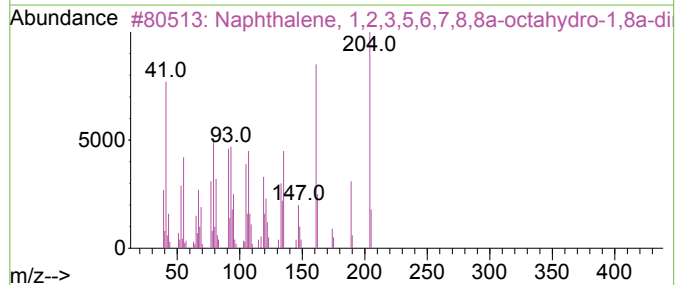
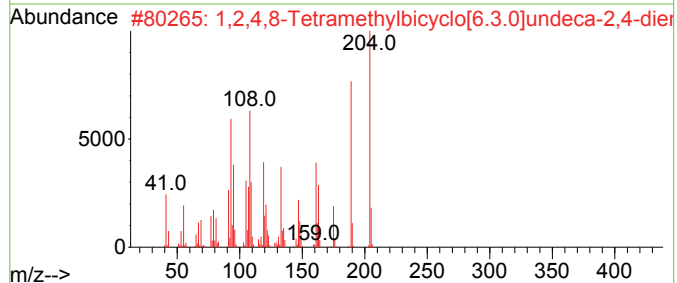
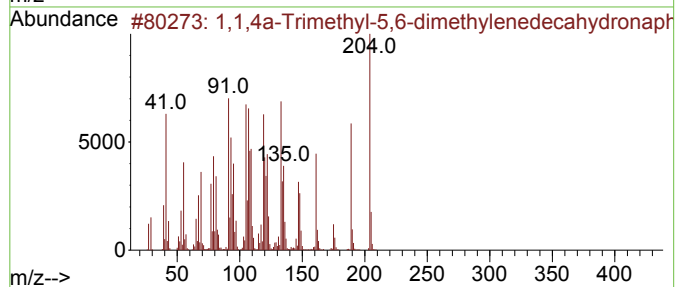
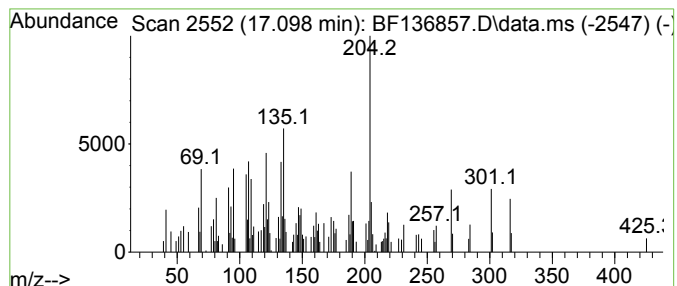
Instrument :
BNA_F
ClientSampleId :
GHL-SS-41

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 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
17.098	5.90 ng	120932	Perylene-d12	15.439		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	52	
2	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	49	
3	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	49	
4	1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	49	
5	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	46	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136857.D
Acq On : 30 Dec 2023 06:48
Operator : CG\JU
Sample : 05897-12
Misc :
ALS Vial : 39 Sample Multiplier: 1

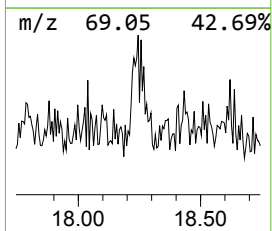
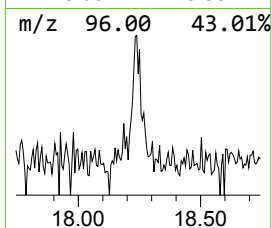
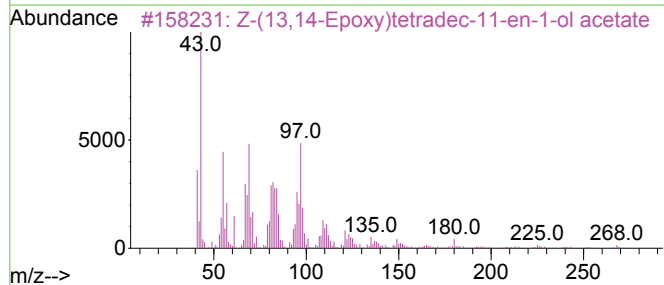
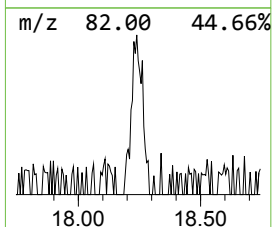
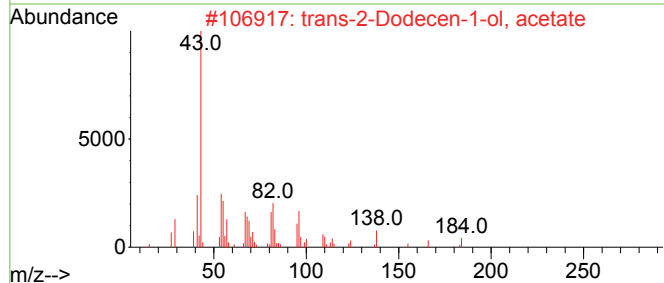
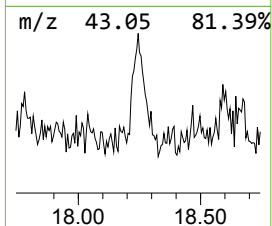
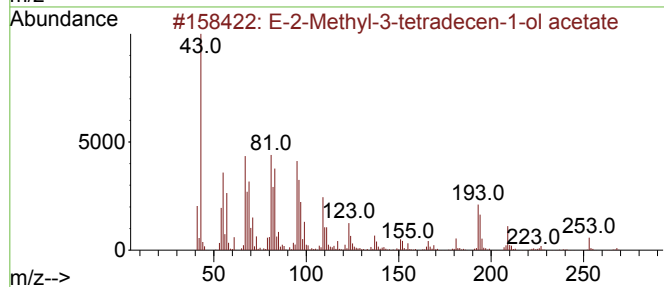
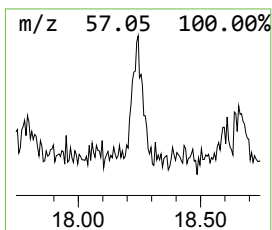
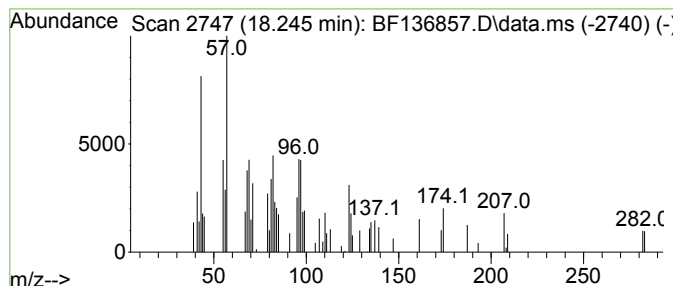
Instrument :
BNA_F
ClientSampleId :
GHL-SS-41

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 unknown18.245 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.245	3.43 ng	70188	Perylene-d12	15.439	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-2-Methyl-3-tetradecen-1-ol ace...	268	C17H32O2	1000130-81-2	38
2	trans-2-Dodecen-1-ol, acetate	226	C14H26O2	084801-16-1	35
3	Z-(13,14-Epoxy)tetradec-11-en-1- ...	268	C16H28O3	1000131-33-2	35
4	Dodecanal	184	C12H24O	000112-54-9	27
5	7-Methyl-Z-8,10-dodecadienal	194	C13H22O	1000130-96-4	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122923\
Data File : BF136857.D
Acq On : 30 Dec 2023 06:48
Operator : CG\JU
Sample : 05897-12
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-41

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
unknown3.322	3.322	4.9	ng	102832	1	6.781	420167	20.0
unknown9.916	9.916	6.4	ng	197214	3	9.810	615614	20.0
Eicosane	15.086	3.3	ng	67489	6	15.439	409665	20.0
Octacosane	15.921	4.2	ng	86942	6	15.439	409665	20.0
Octadecanal	16.745	2.4	ng	49603	6	15.439	409665	20.0
1,1,4a-Trimethy...	17.098	5.9	ng	120932	6	15.439	409665	20.0
unknown18.245	18.245	3.4	ng	70188	6	15.439	409665	20.0