

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
 Data File : BF126101.D
 Acq On : 10 Nov 2021 11:38
 Operator : JU/CG
 Sample : M4475-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB01A

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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126101.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	5	14	20	rBV	2107386	2719733	51.67%	6.732%
2	5.475	571	576	579	rBV	5125828	4888517	92.87%	12.101%
3	6.481	742	747	750	rBV	4539445	4968469	94.39%	12.299%
4	6.851	806	810	814	rBV	1553994	1191795	22.64%	2.950%
5	7.416	900	906	909	rBV	3525396	3270099	62.12%	8.095%
6	8.033	1008	1011	1020	rBV	323584	355529	6.75%	0.880%
7	8.133	1024	1028	1031	rBV	1814618	1435023	27.26%	3.552%
8	9.210	1206	1211	1214	rBV	6572657	5263763	100.00%	13.030%
9	9.551	1265	1269	1271	rBV	98632	90074	1.71%	0.223%
10	9.886	1322	1326	1329	rBV	1886397	1536186	29.18%	3.803%
11	10.674	1455	1460	1463	rBV2	3415363	3285512	62.42%	8.133%
12	11.033	1518	1521	1525	rVB3	80050	87418	1.66%	0.216%
13	11.233	1550	1555	1559	rBV4	85797	100045	1.90%	0.248%
14	11.369	1574	1578	1581	rBV	1489450	1295285	24.61%	3.206%
15	11.392	1581	1582	1586	rVV	184216	123757	2.35%	0.306%
16	11.445	1586	1591	1594	rVB	58811	75244	1.43%	0.186%
17	11.769	1637	1646	1650	rBV	82829	98347	1.87%	0.243%
18	11.863	1659	1662	1665	rBV2	106693	133774	2.54%	0.331%
19	11.904	1665	1669	1672	rVB	368260	376155	7.15%	0.931%
20	12.074	1696	1698	1709	rVB10	57514	93263	1.77%	0.231%
21	12.474	1760	1766	1768	rBV2	133249	146529	2.78%	0.363%
22	12.580	1778	1784	1787	rBV	398105	380261	7.22%	0.941%
23	12.810	1817	1823	1826	rBV	337070	312335	5.93%	0.773%
24	12.957	1844	1848	1851	rBV	4361442	3453930	65.62%	8.550%
25	13.862	1998	2002	2008	rVB2	251572	306274	5.82%	0.758%
26	14.004	2022	2026	2029	rBV2	1168444	1256357	23.87%	3.110%
27	14.033	2029	2031	2033	rVB	158710	123839	2.35%	0.307%
28	14.486	2106	2108	2112	rBV5	80793	127495	2.42%	0.316%
29	14.868	2170	2173	2179	rVB	360459	379822	7.22%	0.940%
30	14.939	2182	2185	2191	rVB2	141241	164130	3.12%	0.406%
31	15.045	2200	2203	2206	rBV	181391	263034	5.00%	0.651%
32	15.133	2215	2218	2220	rBV	139312	140489	2.67%	0.348%
33	15.162	2220	2223	2228	rVB3	218578	285372	5.42%	0.706%
34	15.345	2252	2254	2260	rVB	135546	181429	3.45%	0.449%
35	15.409	2262	2265	2269	rVB	133706	158017	3.00%	0.391%
36	15.474	2272	2276	2279	rBV	767963	889458	16.90%	2.202%

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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-BF110321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.715	2313	2317	2321	rBV2	185841	246610	4.69%	0.610%
38	15.951	2354	2357	2363	rVB2	129159	193927	3.68%	0.480%

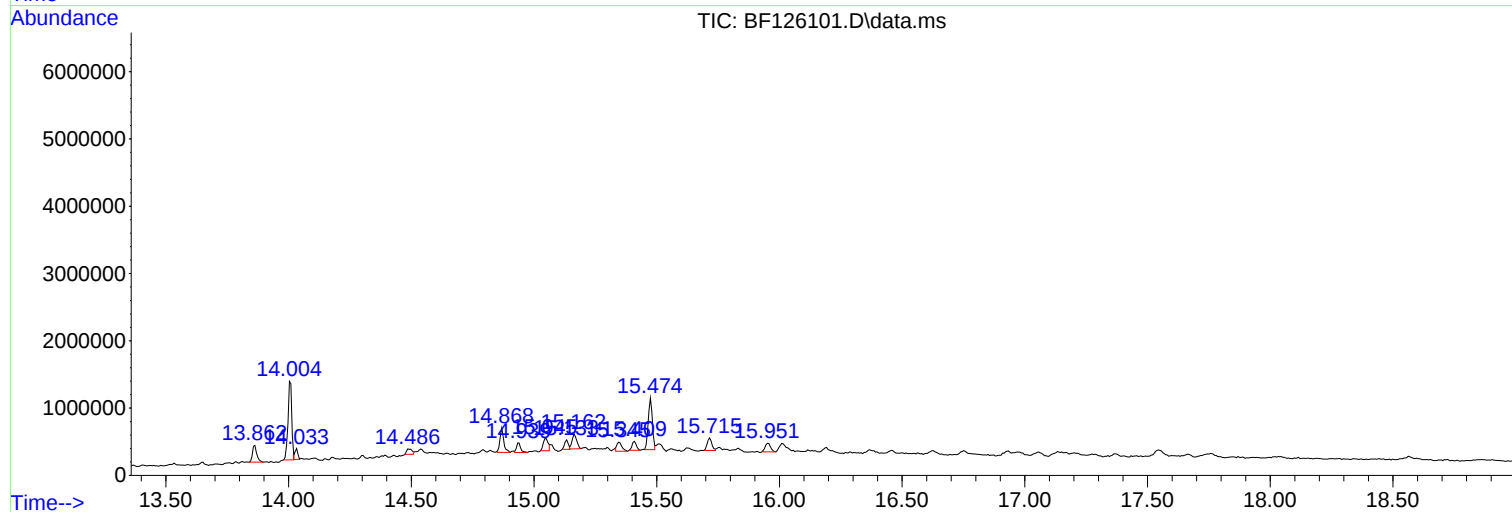
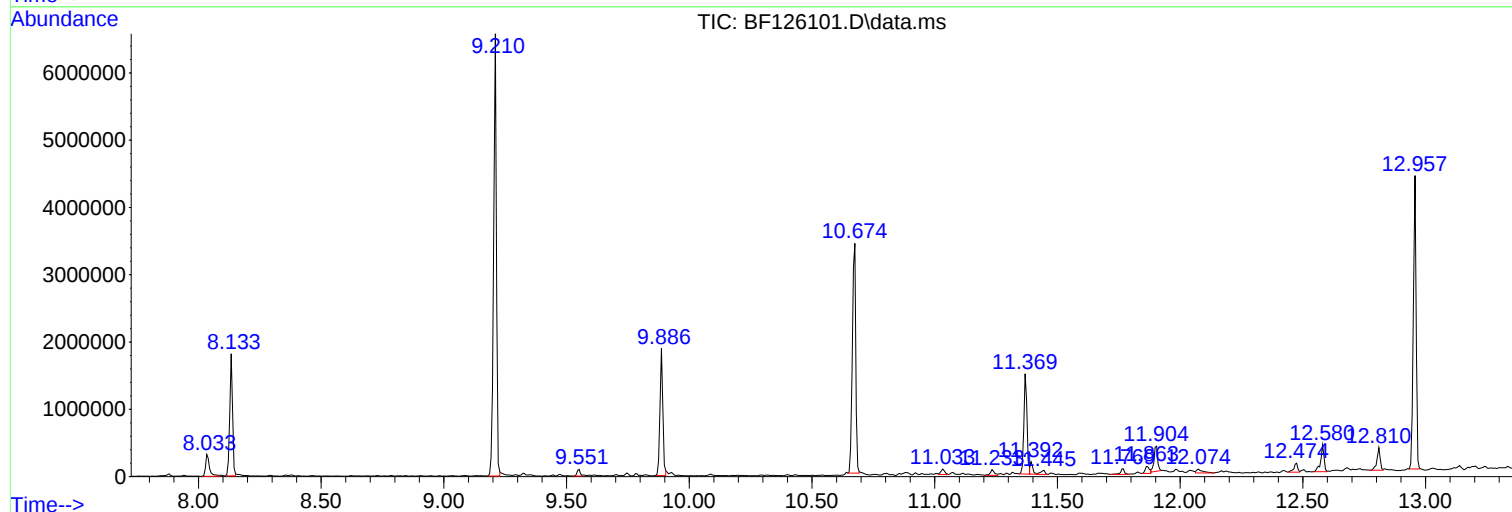
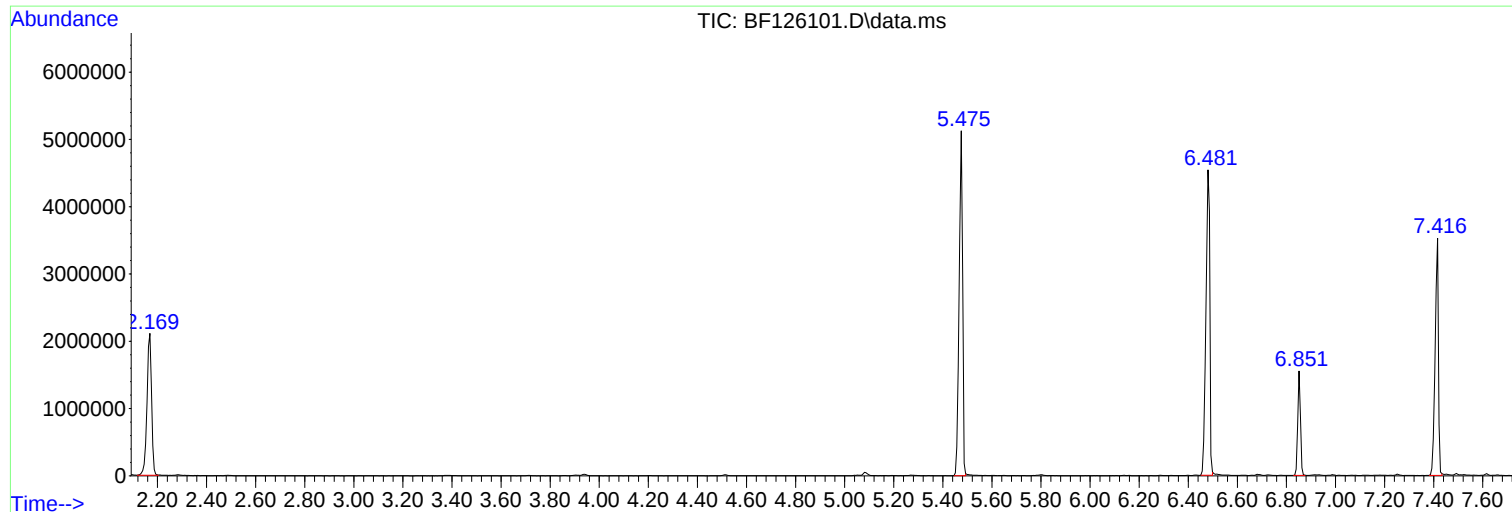
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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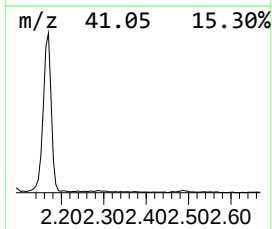
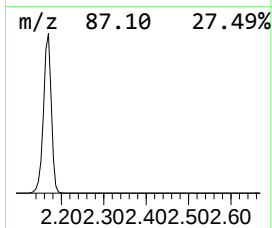
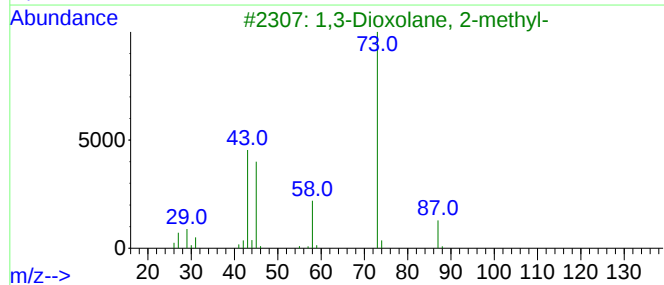
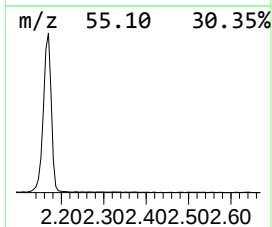
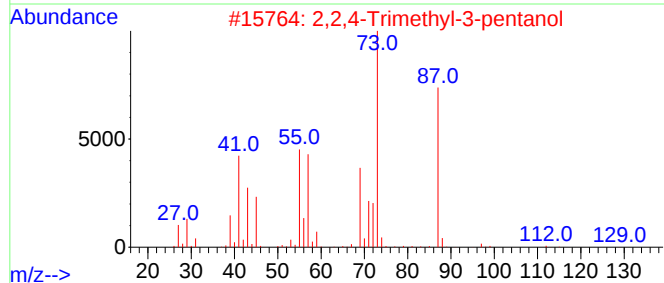
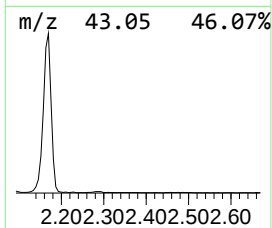
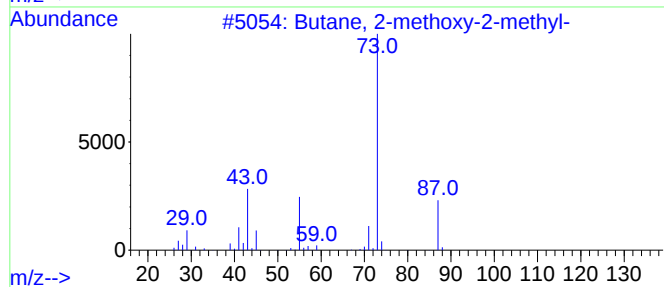
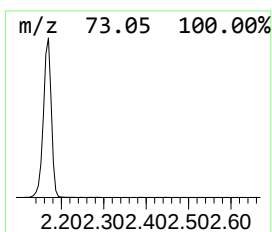
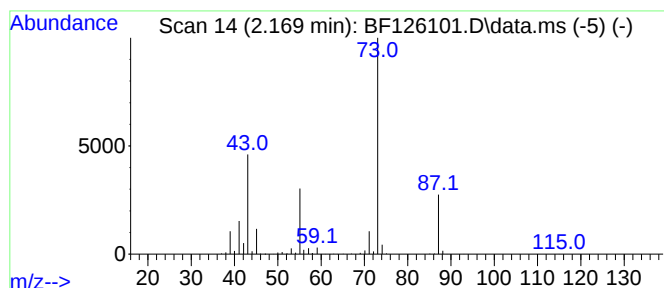
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	45.64 ng	2719730	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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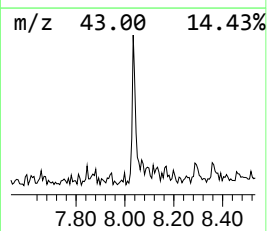
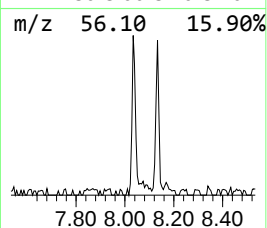
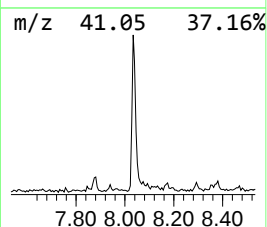
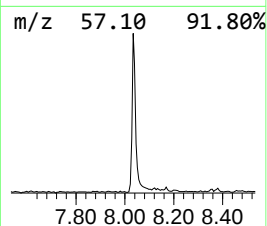
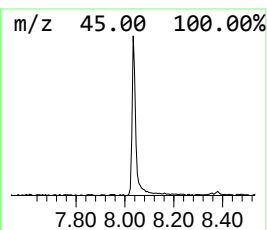
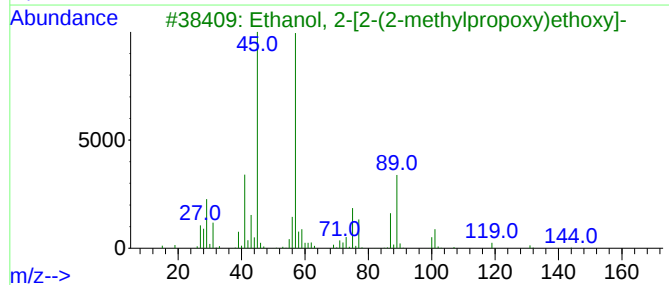
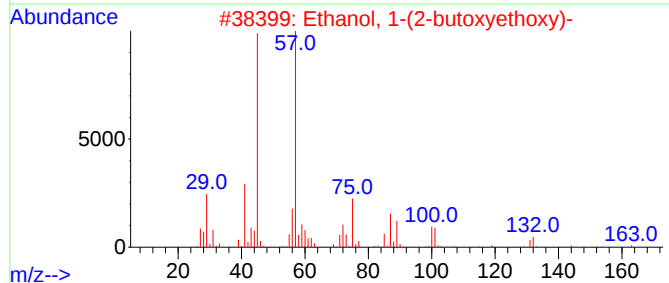
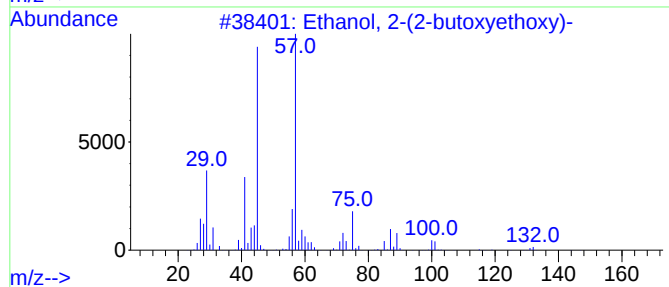
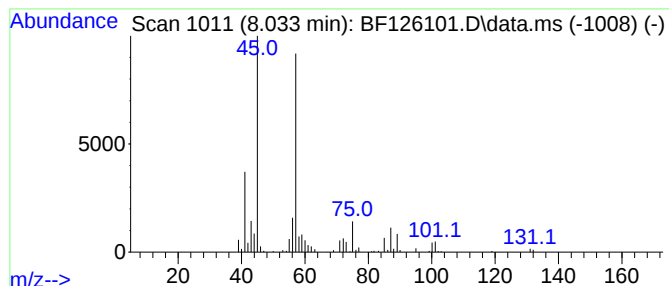
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.033	4.96 ng	355529	Naphthalene-d8	8.133

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	50
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50



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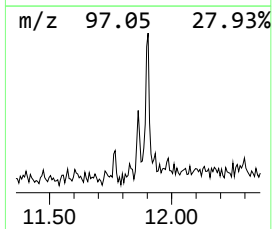
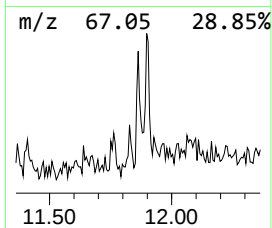
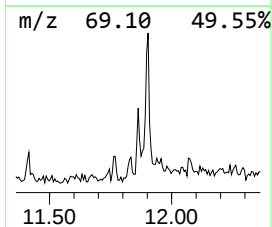
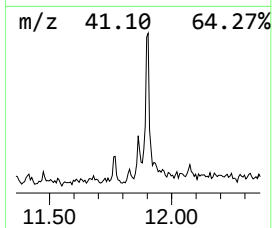
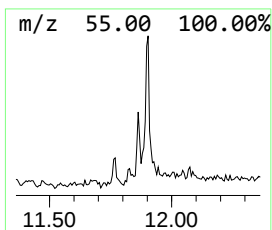
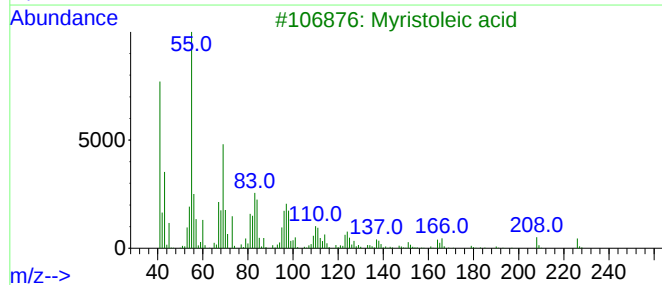
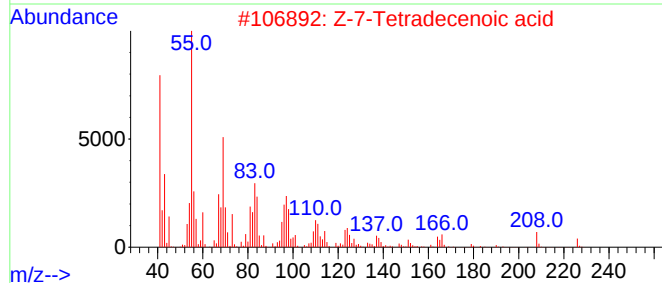
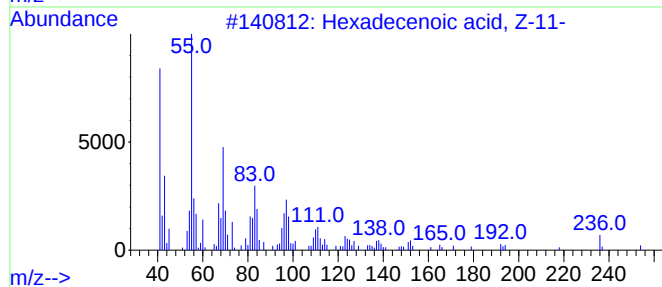
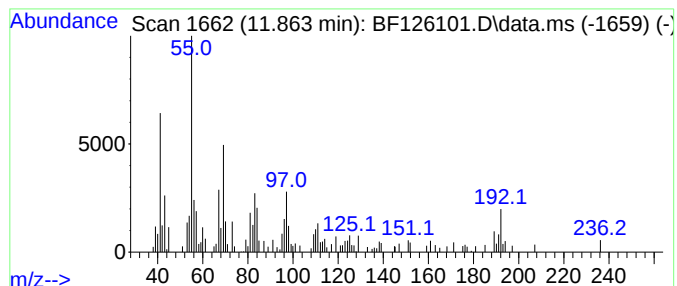
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Hexadecenoic acid, Z-11- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.863	2.07 ng	133774	Phenanthrene-d10		11.368	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecenoic acid, Z-11-		254	C16H30O2	002416-20-8	58
2	Z-7-Tetradecenoic acid		226	C14H26O2	1000130-98-4	49
3	Myristoleic acid		226	C14H26O2	000544-64-9	46
4	E-9-Tetradecenoic acid		226	C14H26O2	050286-30-1	46
5	Palmitoleic acid		254	C16H30O2	000373-49-9	46



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ClientSampleId :
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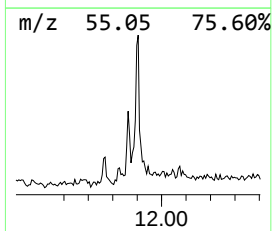
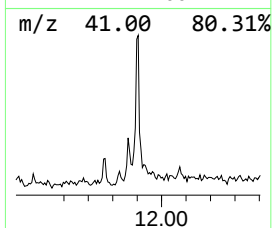
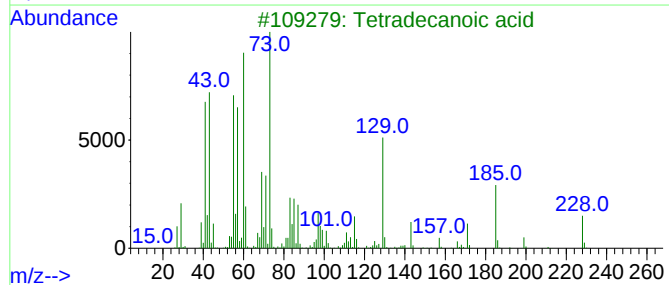
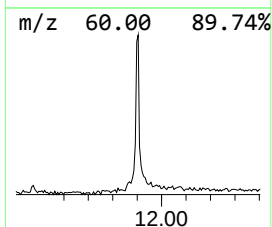
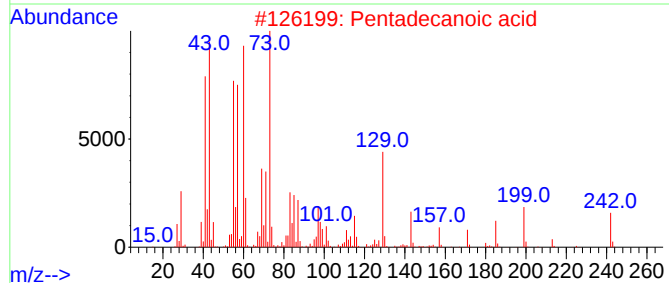
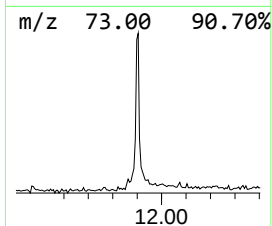
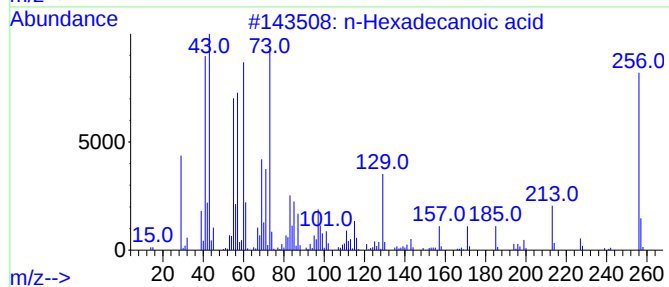
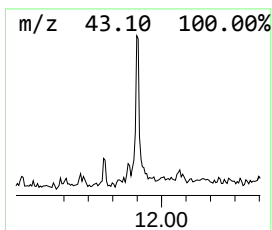
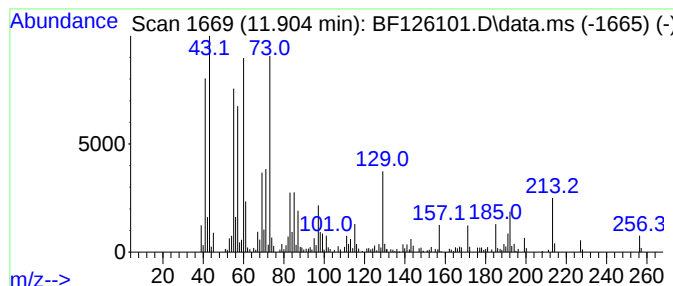
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	5.81 ng	376155	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Undecanoic acid	186	C11H22O2	000112-37-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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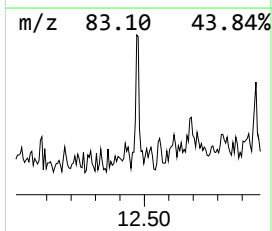
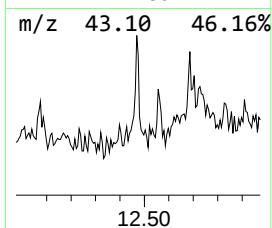
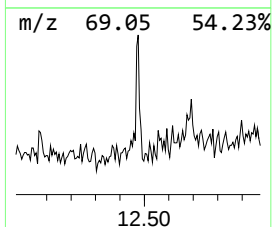
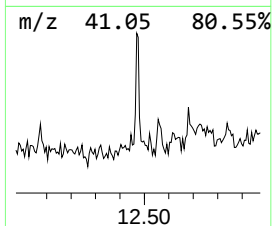
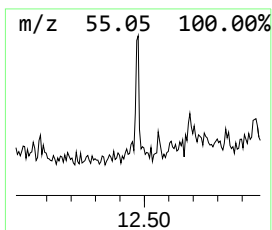
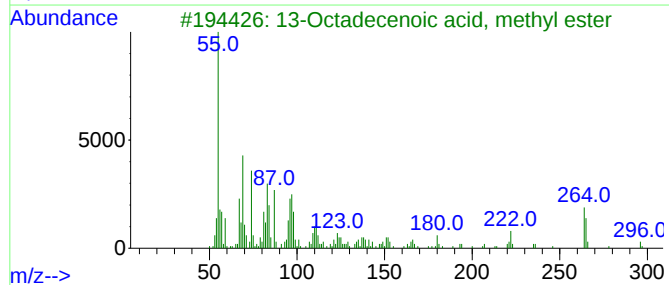
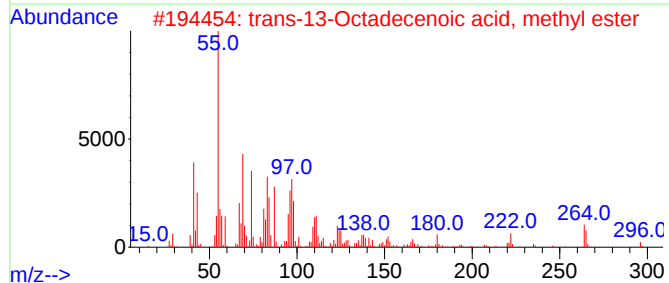
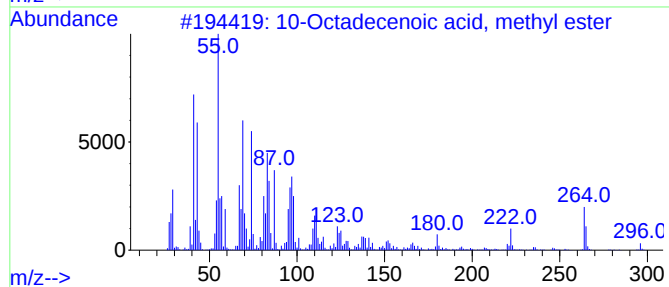
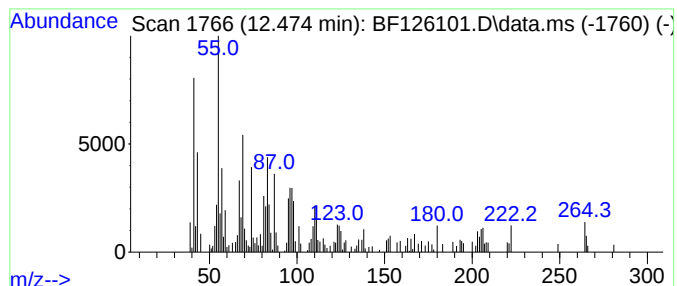
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 10-Octadecenoic acid, methyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.474	2.26 ng	146529	Phenanthrene-d10	11.368

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	81
2			trans-13-Octadecenoic acid, methyl ester	296	C19H36O2	1000333-61-3	81
3			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	72
4			7-Hexadecenoic acid, methyl ester	268	C17H32O2	056875-67-3	68
5			9-Hexadecenoic acid, methyl ester	268	C17H32O2	001120-25-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126101.D
Acq On : 10 Nov 2021 11:38
Operator : JU/CG
Sample : M4475-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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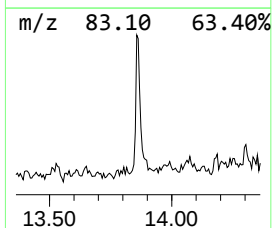
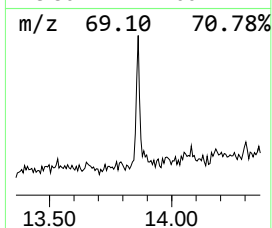
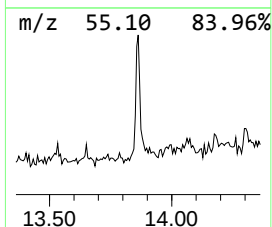
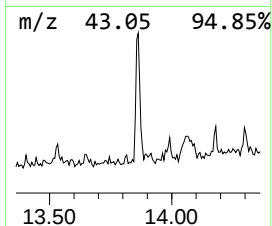
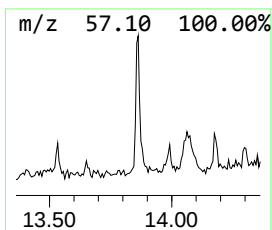
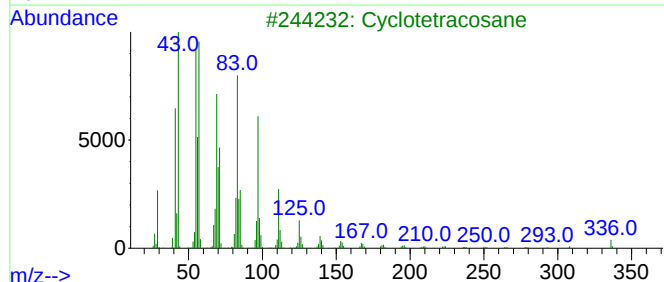
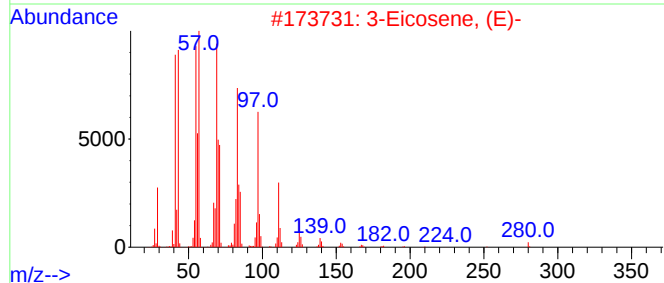
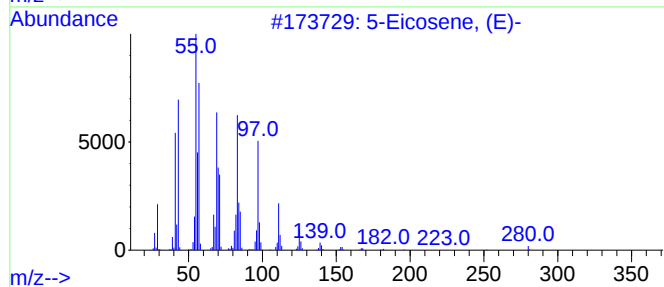
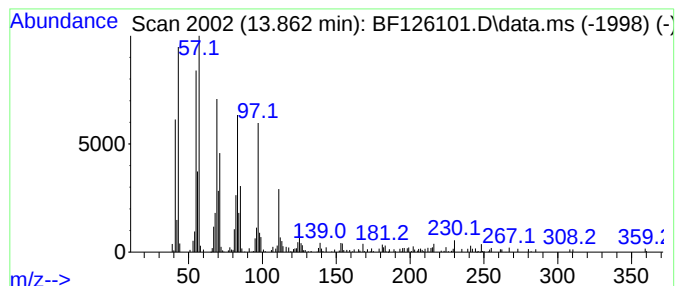
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	4.88 ng	306274	Chrysene-d12	14.009

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	92
2			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3			Cyclotetracosane	336	C24H48	000297-03-0	90
4			Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	90
5			1-Eicosene	280	C20H40	003452-07-1	90



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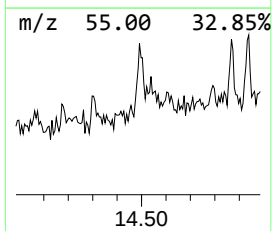
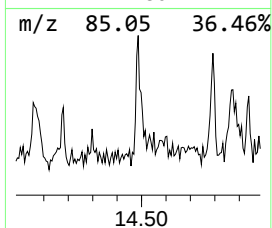
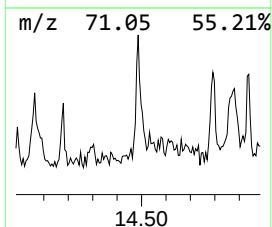
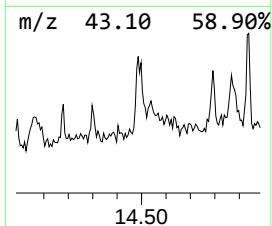
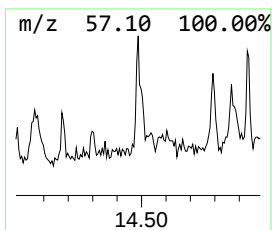
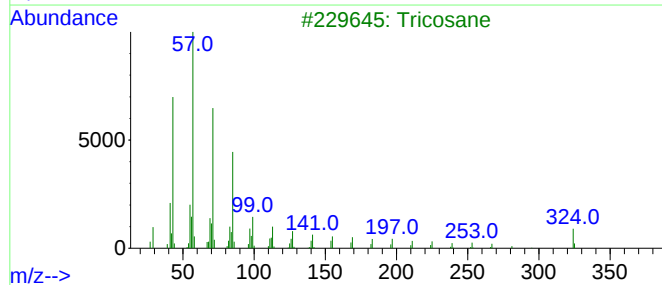
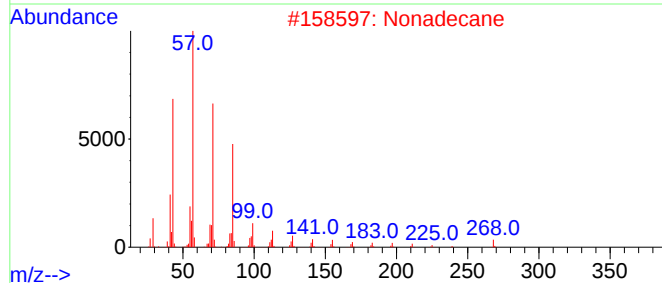
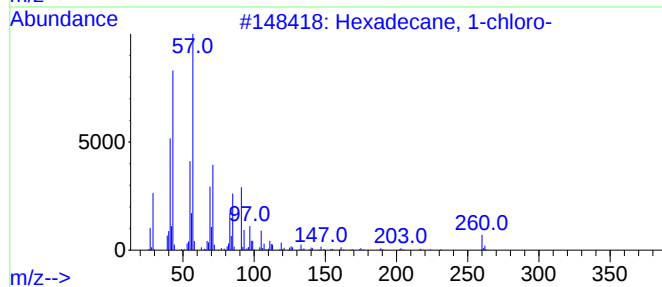
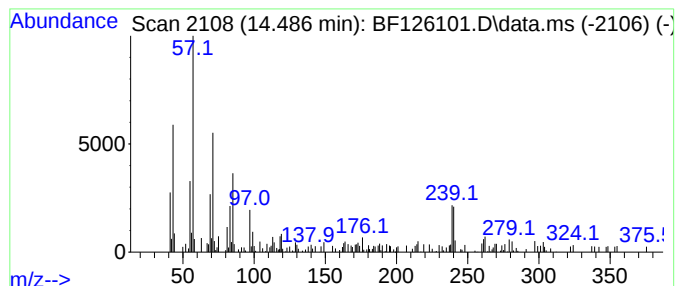
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.486 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.486	2.03 ng	127495	Chrysene-d12	14.009	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	46
2	Nonadecane	268	C19H40	000629-92-5	42
3	Tricosane	324	C23H48	000638-67-5	41
4	Octacosane	394	C28H58	000630-02-4	41
5	Tetratetracontane	619	C44H90	007098-22-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126101.D
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Sample : M4475-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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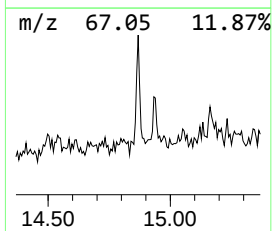
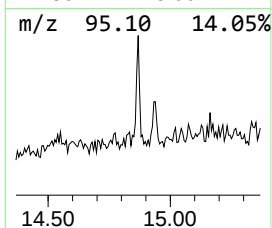
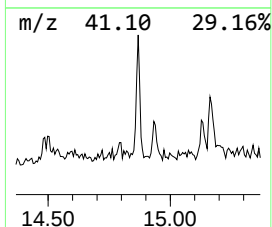
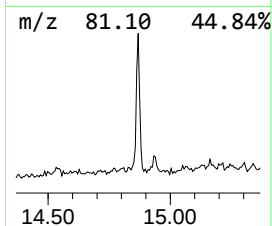
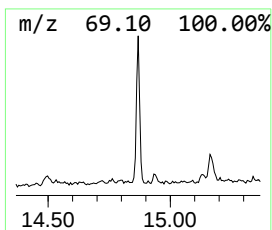
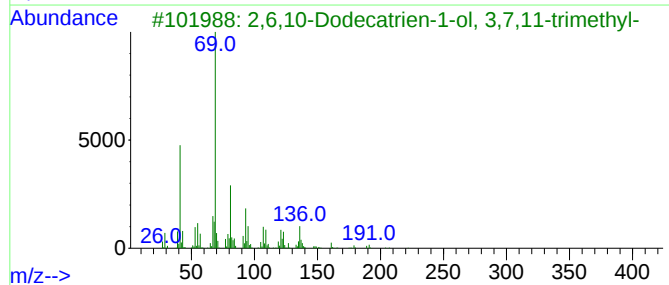
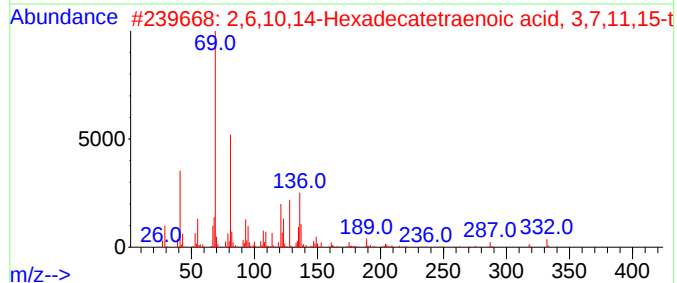
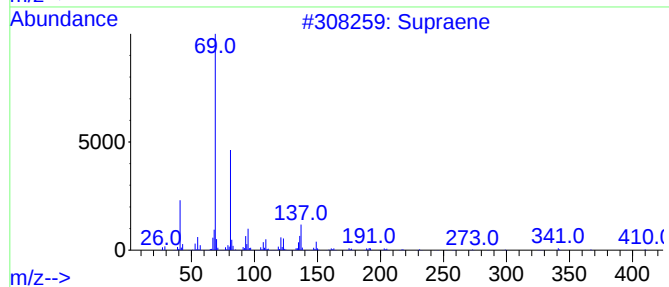
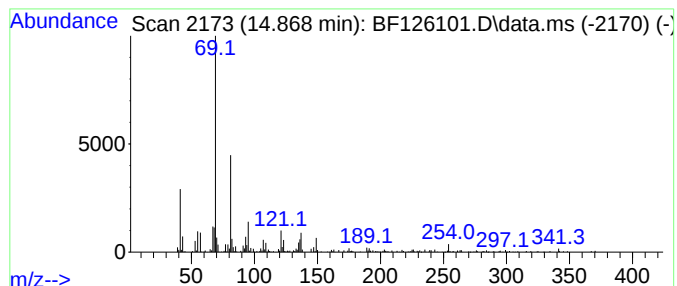
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	8.54 ng	379822	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
3			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
5			4-Oxo-.beta.-damascone	206	C13H18O2	053398-08-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126101.D
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Misc :
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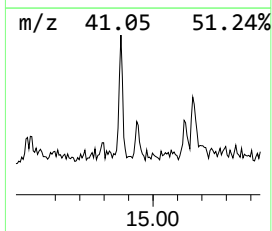
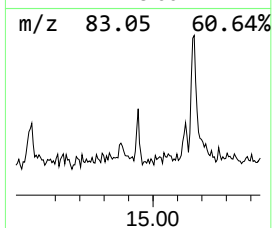
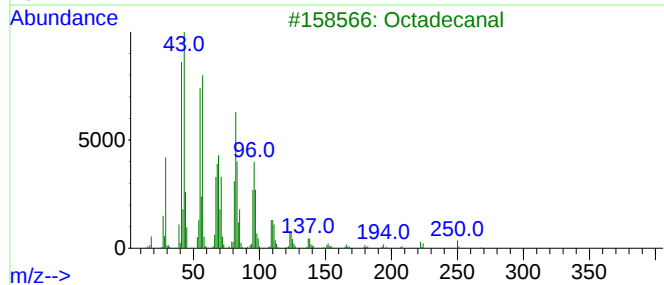
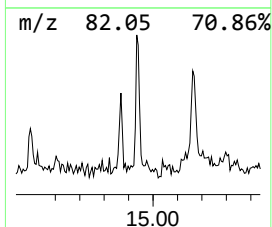
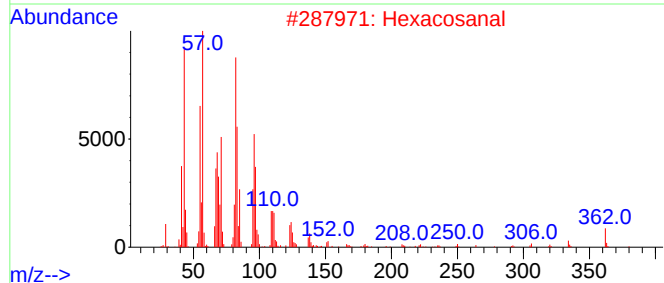
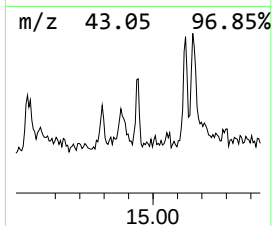
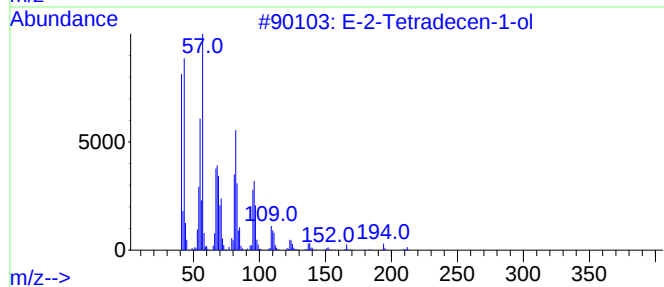
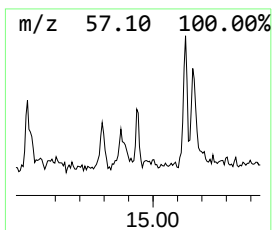
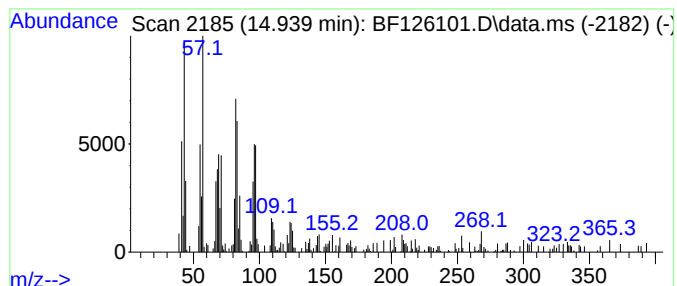
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 E-2-Tetradecen-1-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	3.69 ng	164130	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-2-Tetradecen-1-ol			212	C14H28O	1000130-83-7	86
2	Hexacosanal			380	C26H52O	026627-85-0	83
3	Octadecanal			268	C18H36O	000638-66-4	76
4	Pentadecanal-			226	C15H30O	002765-11-9	70
5	Hexadecanal			240	C16H32O	000629-80-1	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
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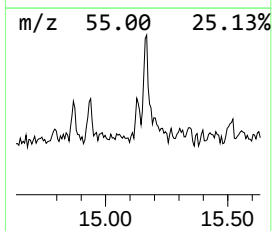
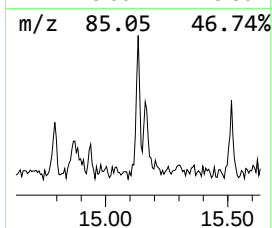
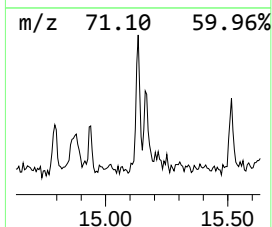
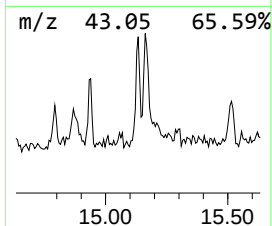
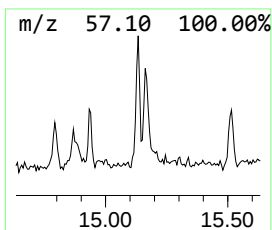
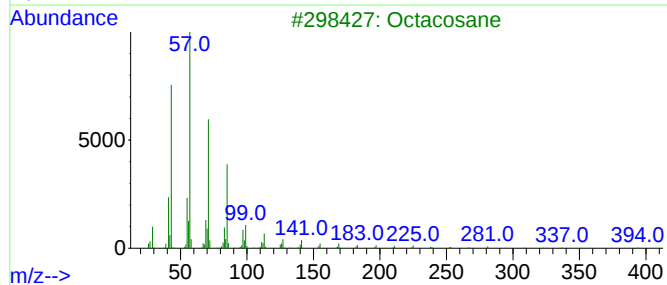
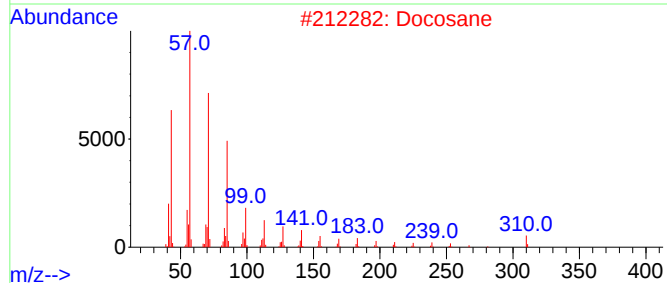
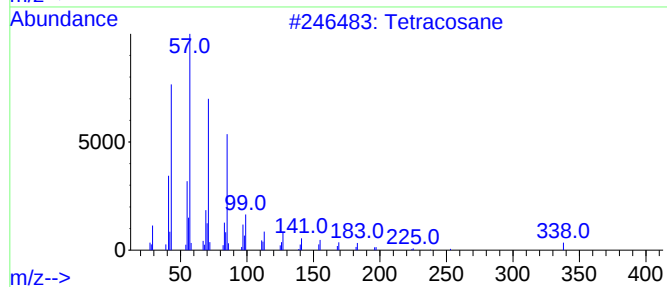
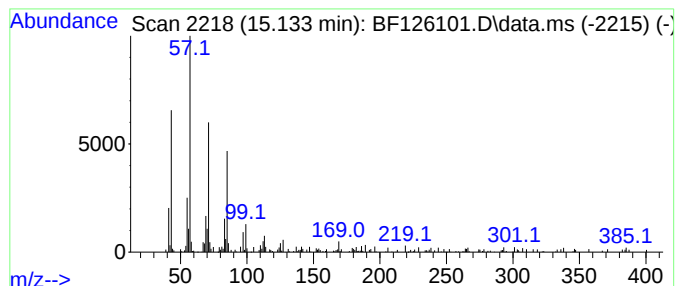
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.133	3.16 ng	140489	Perylene-d12	15.474	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	93
2	Docosane	310	C22H46	000629-97-0	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Heneicosane	296	C21H44	000629-94-7	86
5	Heptacosane	380	C27H56	000593-49-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
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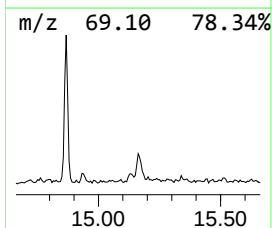
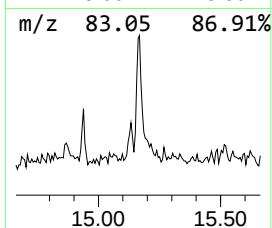
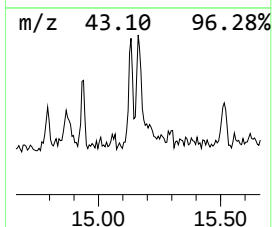
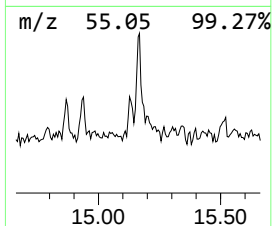
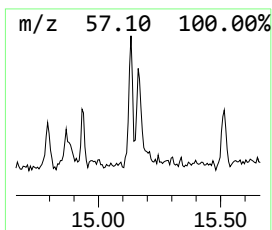
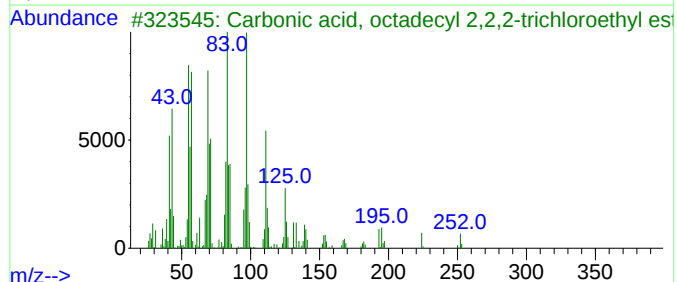
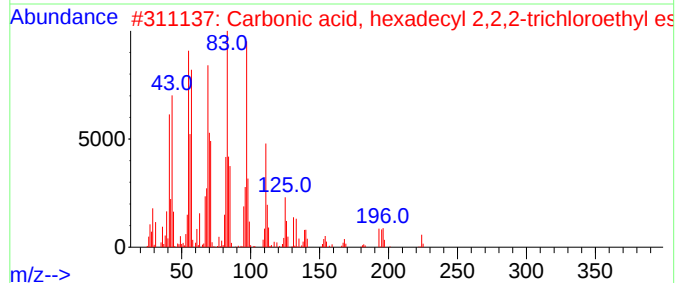
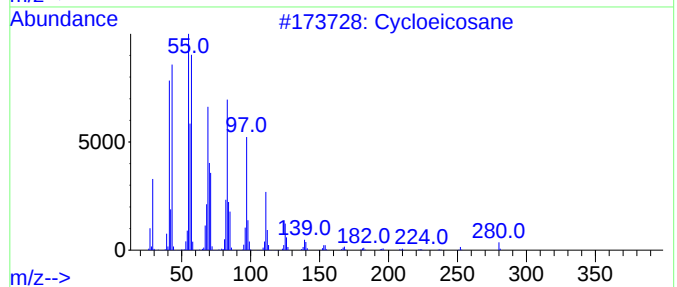
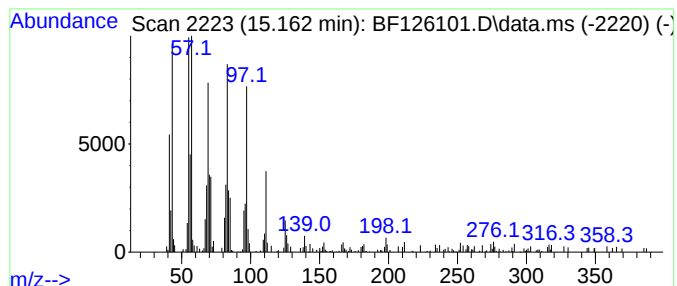
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Cycloeicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.162	6.42 ng	285372	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	93
2			Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	91
3			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
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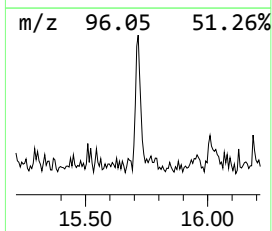
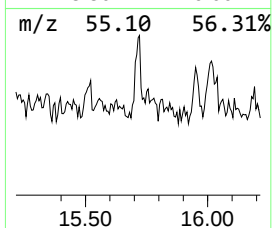
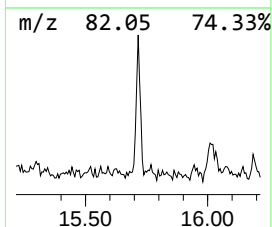
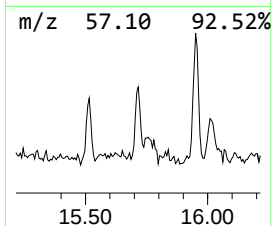
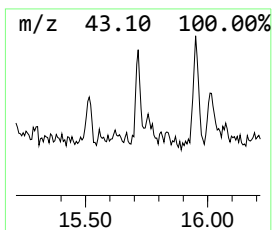
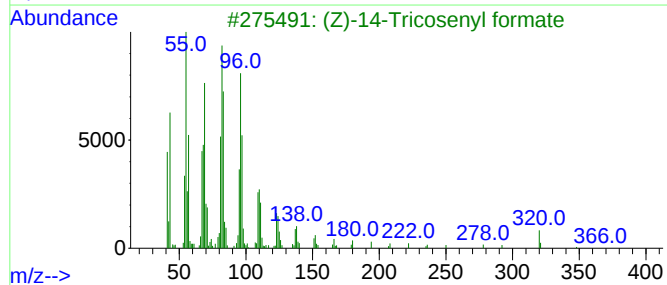
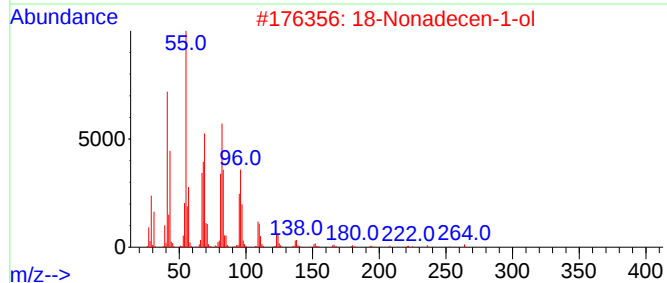
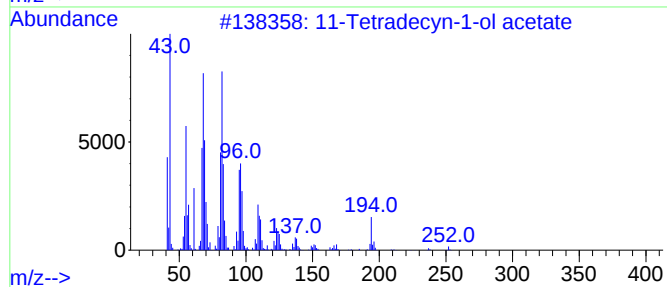
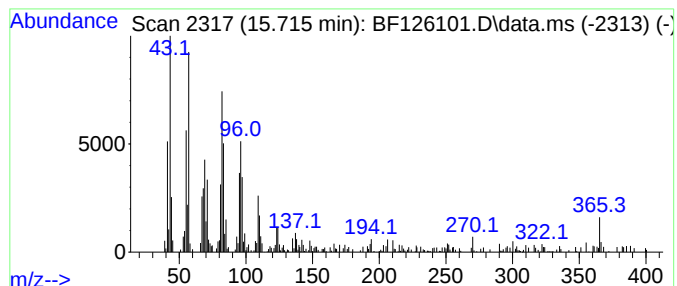
Instrument :
BNA_F
ClientSampleId :
SB01A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 11-Tetradecyn-1-ol acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.715	5.55 ng	246610	Perylene-d12	15.474	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tetradecyn-1-ol acetate	252	C16H28O2	033925-72-3	87
2	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	83
3	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	83
4	11-Eicosenol	296	C20H40O	1010424-20-3	80
5	1,7-Hexadecadiene	222	C16H30	125110-62-5	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126101.D
Acq On : 10 Nov 2021 11:38
Operator : JU/CG
Sample : M4475-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB01A

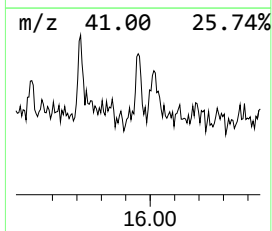
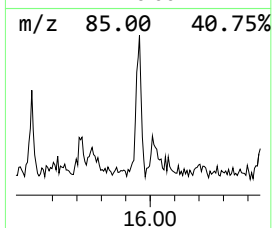
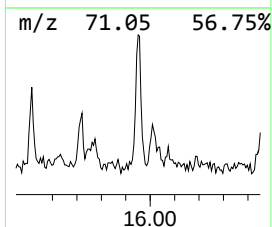
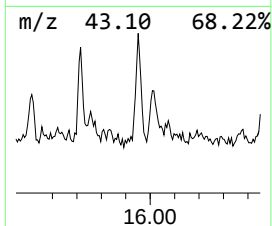
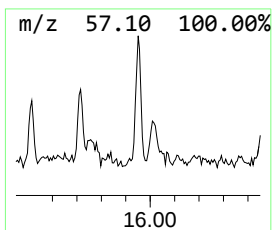
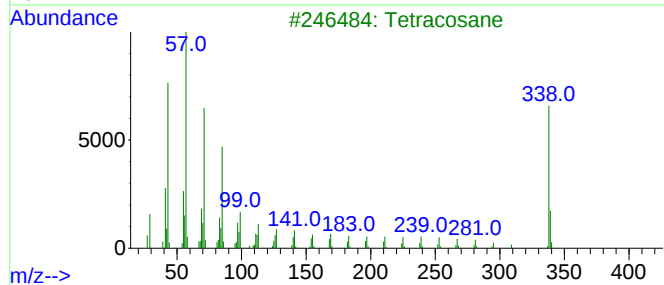
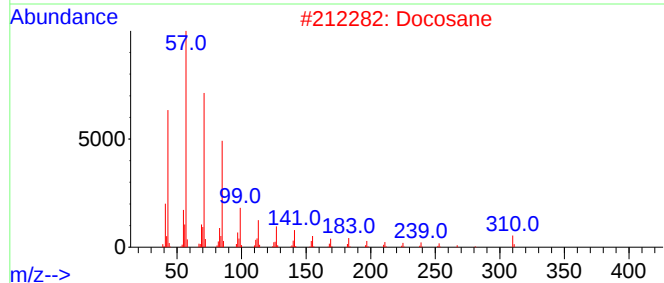
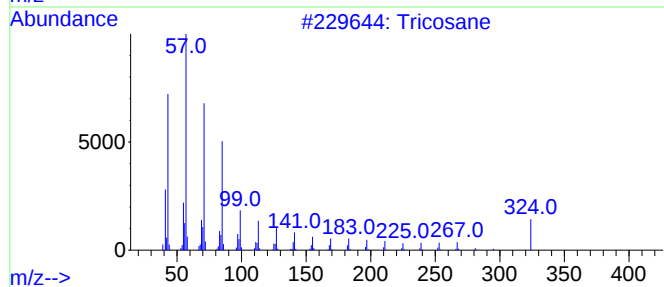
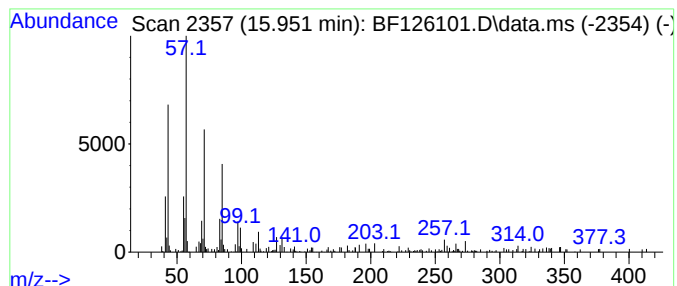
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tricosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	4.36 ng	193927	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosane	324	C23H48	000638-67-5	76
2			Docosane	310	C22H46	000629-97-0	76
3			Tetracosane	338	C24H50	000646-31-1	76
4			Heptacosane	380	C27H56	000593-49-7	68
5			Nonadecane	268	C19H40	000629-92-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111021\
Data File : BF126101.D
Acq On : 10 Nov 2021 11:38
Operator : JU/CG
Sample : M4475-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB01A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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
Butane, 2-metho...	2.169	45.6	ng	2719730	1	6.851	1191800	20.0
Ethanol, 2-(2-b...	8.033	5.0	ng	355529	2	8.133	1435020	20.0
Hexadecenoic ac...	11.863	2.1	ng	133774	4	11.368	1295290	20.0
n-Hexadecanoic ...	11.904	5.8	ng	376155	4	11.368	1295290	20.0
10-Octadecenoic...	12.474	2.3	ng	146529	4	11.368	1295290	20.0
5-Eicosene, (E)-	13.863	4.9	ng	306274	5	14.009	1256360	20.0
unknown14.486	14.486	2.0	ng	127495	5	14.009	1256360	20.0
Supraene	14.868	8.5	ng	379822	6	15.474	889458	20.0
E-2-Tetradecen-...	14.939	3.7	ng	164130	6	15.474	889458	20.0
Tetracosane	15.133	3.2	ng	140489	6	15.474	889458	20.0
Cycloeicosane	15.162	6.4	ng	285372	6	15.474	889458	20.0
11-Tetradecyn-1...	15.715	5.5	ng	246610	6	15.474	889458	20.0
Tricosane	15.951	4.4	ng	193927	6	15.474	889458	20.0