

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
 Data File : BF137435.D
 Acq On : 28 Feb 2024 21:19
 Operator : CG\JU
 Sample : P1538-11
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20241104-AMENDED-COMPOSITE-35N-N-4-03

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-BF022324.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137435.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.992	489	494	508	rBV	1402120	1445499	28.60%	5.001%
2	5.404	561	564	592	rBV	1843959	1813256	35.88%	6.273%
3	6.416	732	736	750	rBV	3260039	3240733	64.12%	11.211%
4	6.781	795	798	806	rBV	917374	793594	15.70%	2.745%
5	6.845	806	809	815	rVV	70372	75826	1.50%	0.262%
6	6.892	815	817	821	rVB	73325	62959	1.25%	0.218%
7	7.339	890	893	906	rBV	2493561	2405832	47.60%	8.323%
8	7.498	917	920	922	rBV	96637	88616	1.75%	0.307%
9	8.057	1012	1015	1025	rBV	1198842	1134272	22.44%	3.924%
10	9.139	1195	1199	1202	rBV	5288087	4408069	87.22%	15.249%
11	9.816	1311	1314	1318	rBV	1755327	1371966	27.15%	4.746%
12	9.922	1328	1332	1337	rVB2	62809	77238	1.53%	0.267%
13	10.610	1445	1449	1457	rBV	1427694	1274742	25.22%	4.410%
14	10.745	1467	1472	1478	rVB4	93355	133957	2.65%	0.463%
15	10.798	1478	1481	1484	rBV	62384	62699	1.24%	0.217%
16	10.939	1502	1505	1509	rVB3	62226	69302	1.37%	0.240%
17	11.180	1543	1546	1549	rBV	286644	236165	4.67%	0.817%
18	11.310	1565	1568	1571	rBV	1805103	1545244	30.57%	5.346%
19	11.927	1669	1673	1678	rBV4	76839	123956	2.45%	0.429%
20	12.533	1773	1776	1779	rVB	222325	170937	3.38%	0.591%
21	12.763	1812	1815	1818	rVB	240443	211845	4.19%	0.733%
22	12.915	1836	1841	1844	rBV	5487151	5053948	100.00%	17.484%
23	13.821	1992	1995	2003	rBV	270966	291254	5.76%	1.008%
24	13.968	2016	2020	2023	rBV	1342322	1359202	26.89%	4.702%
25	14.457	2101	2103	2106	rBV3	68039	61595	1.22%	0.213%
26	15.021	2196	2199	2207	rVB	80528	142601	2.82%	0.493%
27	15.327	2248	2251	2258	rVB	64651	97098	1.92%	0.336%
28	15.392	2259	2262	2268	rVV	77122	104023	2.06%	0.360%
29	15.457	2268	2273	2281	rVV	853392	1050405	20.78%	3.634%

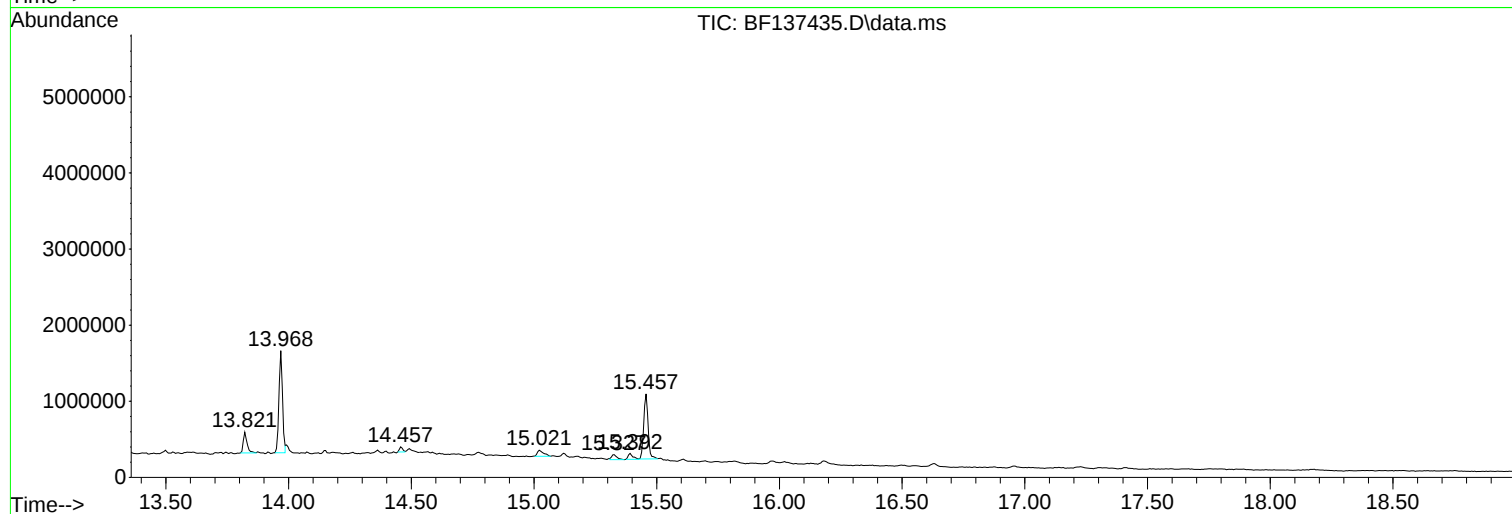
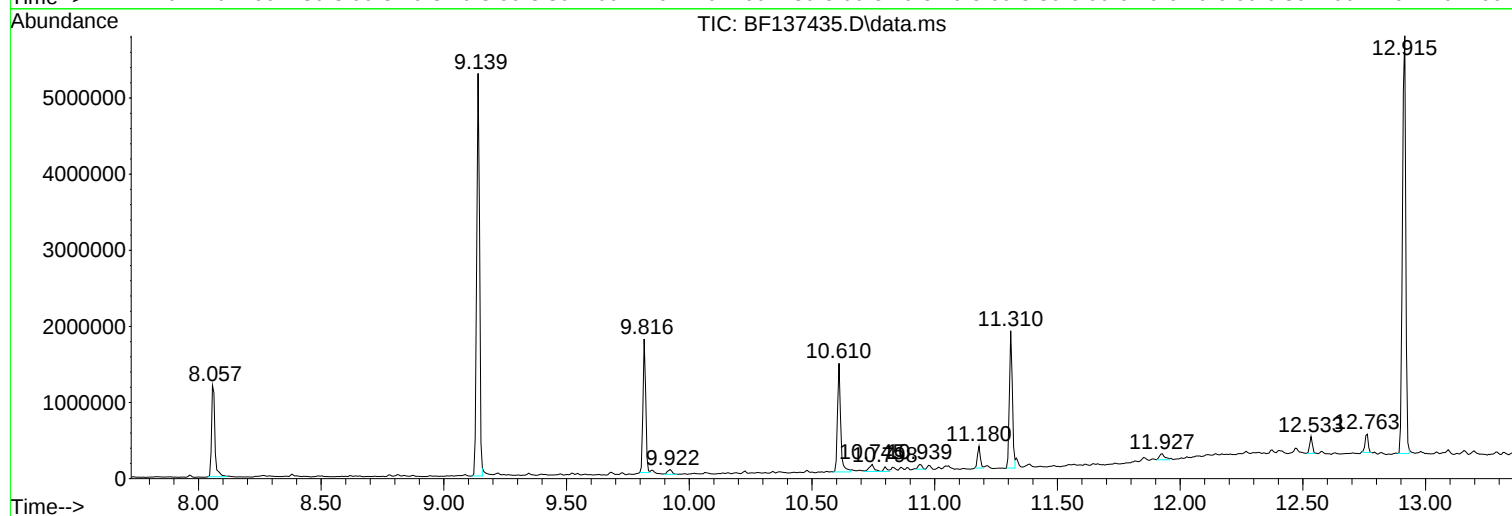
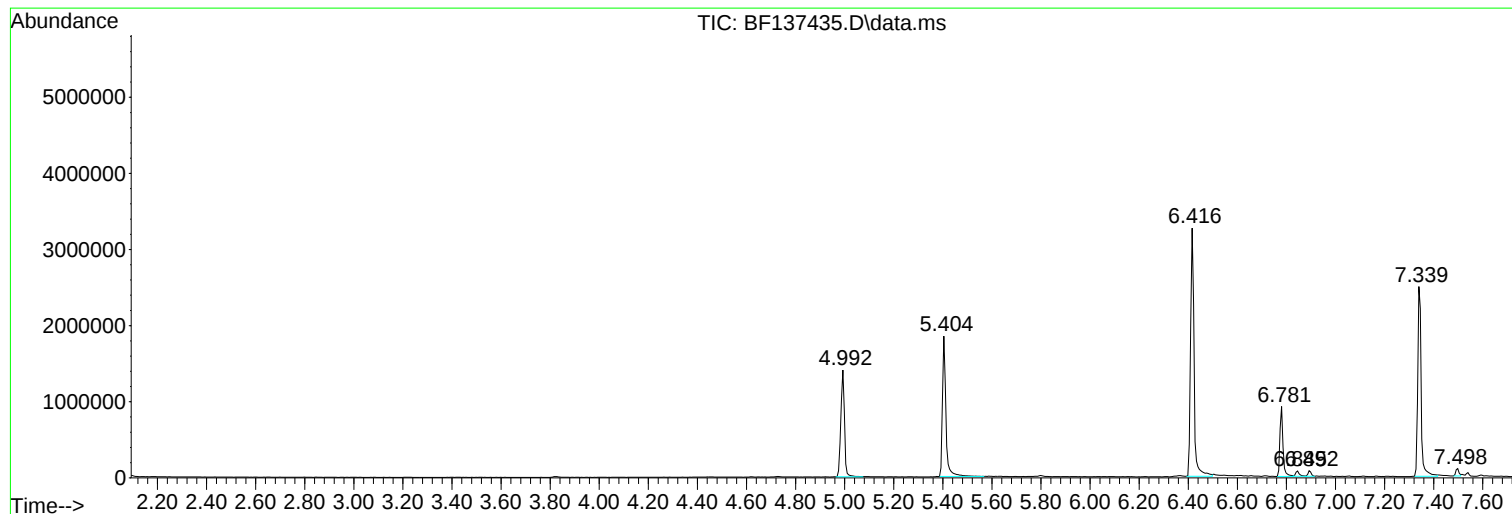
Sum of corrected areas: 28906833

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
Data File : BF137435.D
Acq On : 28 Feb 2024 21:19
Operator : CG\JU
Sample : P1538-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20241104-AMENDED-COMPOSITE-35N-N-4-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
Data File : BF137435.D
Acq On : 28 Feb 2024 21:19
Operator : CG\JU
Sample : P1538-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :

BNA_F

ClientSampleId :

20241104-AMENDED-COMPOSITE-35N-N-4-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M

Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

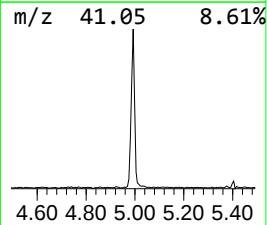
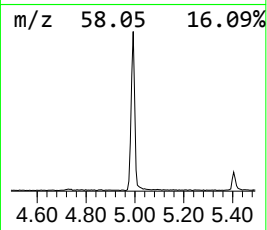
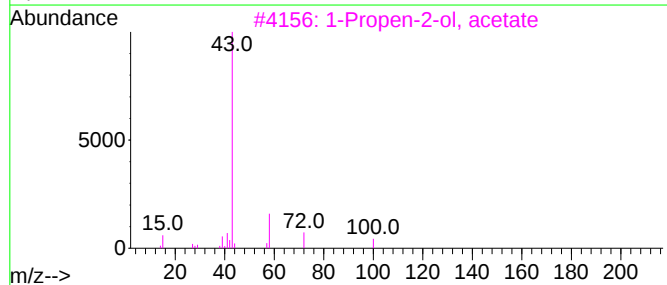
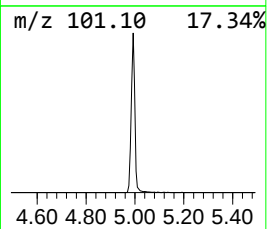
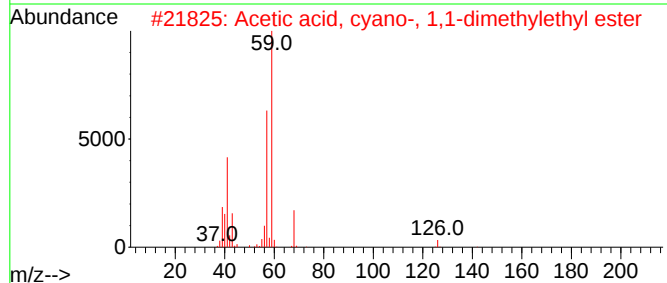
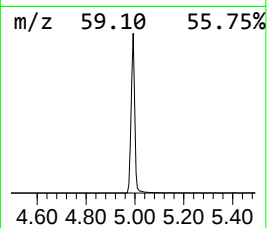
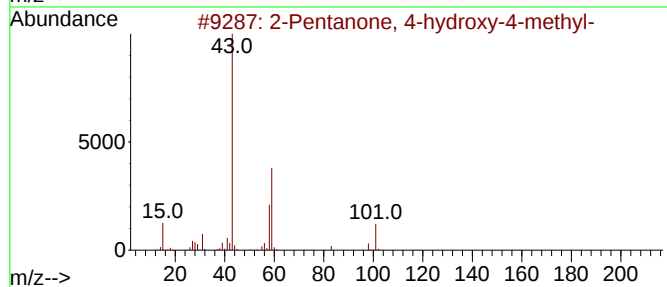
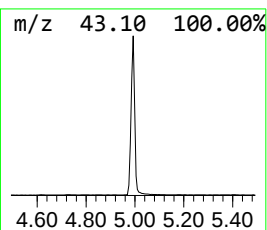
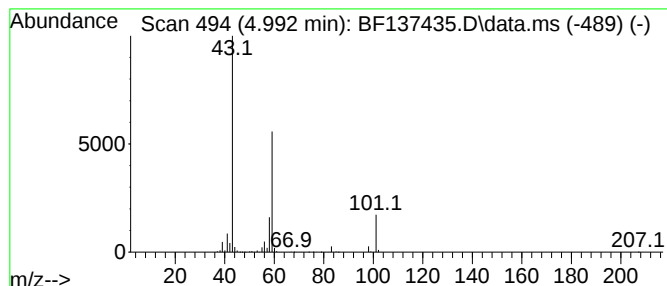
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.992	36.43 ng	1445500	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
Data File : BF137435.D
Acq On : 28 Feb 2024 21:19
Operator : CG\JU
Sample : P1538-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :

BNA_F

ClientSampleId :

20241104-AMENDED-COMPOSITE-35N-N-4-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M

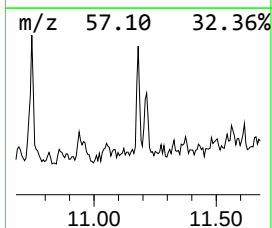
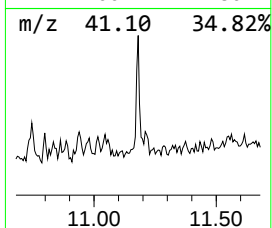
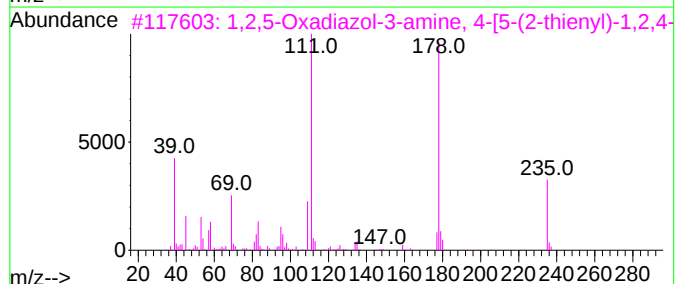
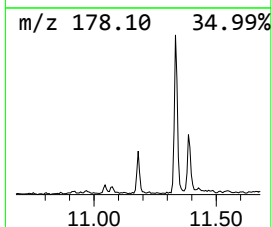
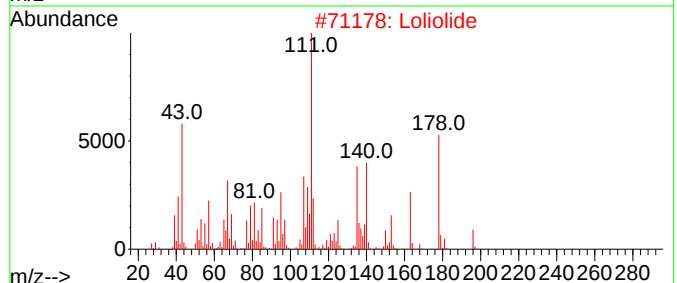
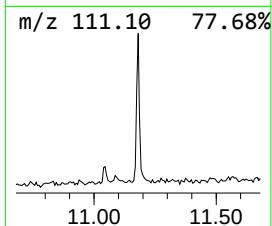
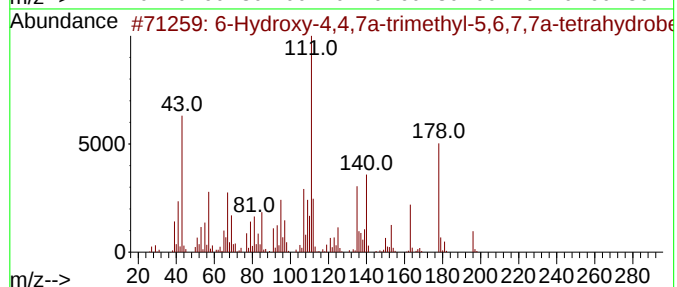
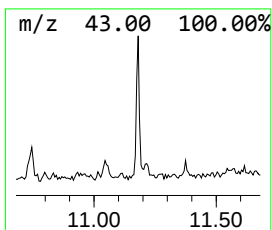
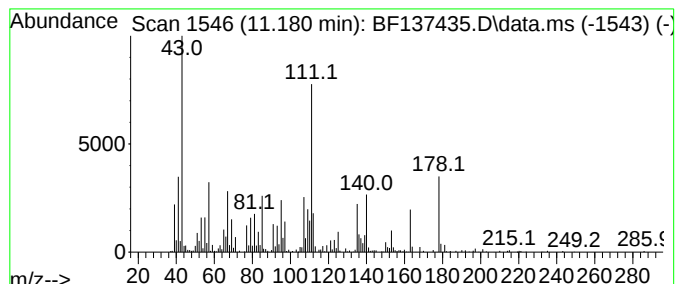
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 6-Hydroxy-4,4,7a-trimethyl-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.180	3.06 ng	236165	Phenanthrene-d10	11.310	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Hydroxy-4,4,7a-trimethyl-5,6,7...	196	C11H16O3	073410-02-3	91
2	Loliolide	196	C11H16O3	005989-02-6	90
3	1,2,5-Oxadiazol-3-amine, 4-[5-(2...	235	C8H5N5O2S	1000277-21-2	38
4	2-Butyl-5-methyl-3-(2-methylprop...	222	C15H26O	1010281-10-6	32
5	(E)-Dodec-5-en-4-olide	196	C12H20O2	1000370-40-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
Data File : BF137435.D
Acq On : 28 Feb 2024 21:19
Operator : CG\JU
Sample : P1538-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :

BNA_F

ClientSampleId :

20241104-AMENDED-COMPOSITE-35N-N-4-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M

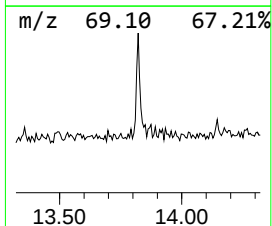
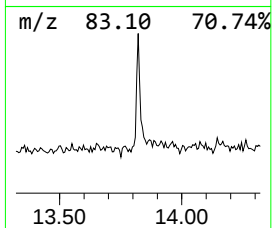
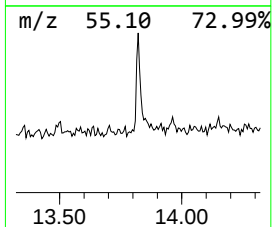
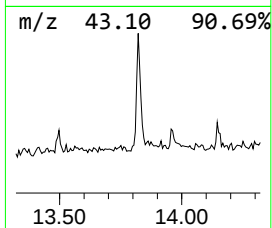
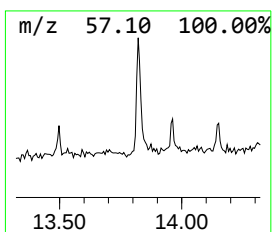
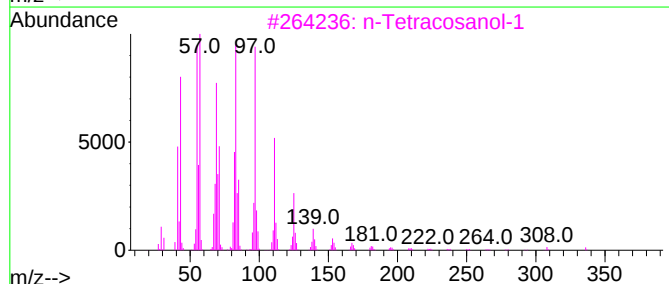
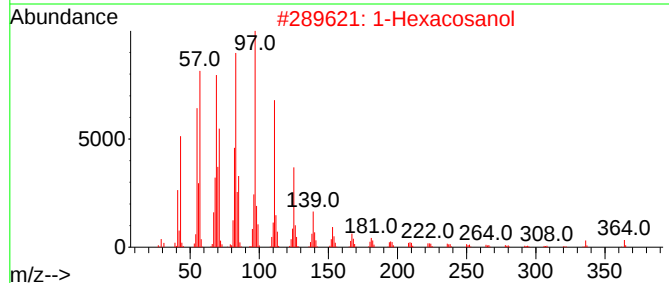
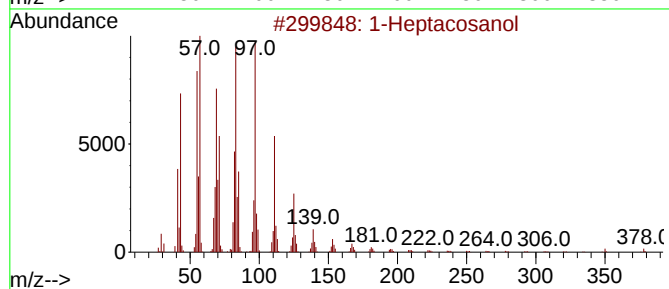
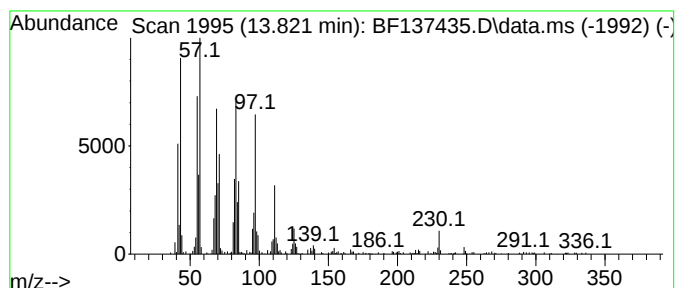
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Heptacosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.821	4.29 ng	291254	Chrysene-d12	13.968	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	1-Hexacosanol	382	C26H54O	000506-52-5	91
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4	Triacontan-15-ol	438	C30H62O	031849-26-0	87
5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022824\
Data File : BF137435.D
Acq On : 28 Feb 2024 21:19
Operator : CG\JU
Sample : P1538-11
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :

BNA_F

ClientSampleId :

20241104-AMENDED-COMPOSITE-35N-N-4-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.992	36.4	ng	1445500	1	6.781	793594	20.0
6-Hydroxy-4,4,7...	11.180	3.1	ng	236165	4	11.310	1545240	20.0
1-Heptacosanol	13.821	4.3	ng	291254	5	13.968	1359200	20.0