

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
 Data File : BF136504.D
 Acq On : 11 Dec 2023 22:28
 Operator : CG\JU
 Sample : 05659-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SU-04-120623

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-BF120523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136504.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	15	19	32	rVB2	38434	71165	2.78%	0.389%
2	5.034	496	501	508	rBV	347363	406430	15.90%	2.220%
3	5.440	565	570	573	rBV	2493956	2200727	86.12%	12.020%
4	6.440	735	740	743	rBV	2200616	2104389	82.35%	11.493%
5	6.628	768	772	783	rBV4	30085	43287	1.69%	0.236%
6	6.793	797	800	807	rVB	861431	664531	26.00%	3.629%
7	7.357	884	896	899	rBV	1517658	1396560	54.65%	7.628%
8	7.610	934	939	944	rVB2	35870	39173	1.53%	0.214%
9	8.069	1012	1017	1021	rBV	1035665	831766	32.55%	4.543%
10	8.387	1069	1071	1075	rBV	31974	38676	1.51%	0.211%
11	9.151	1196	1201	1204	rBV	2983638	2555424	100.00%	13.957%
12	9.228	1211	1214	1219	rVB	44947	47455	1.86%	0.259%
13	9.551	1264	1269	1271	rBV4	33563	37190	1.46%	0.203%
14	9.763	1303	1305	1309	rVB	34508	29065	1.14%	0.159%
15	9.828	1312	1316	1319	rVB	935411	752026	29.43%	4.107%
16	9.934	1330	1334	1337	rVB4	25526	34536	1.35%	0.189%
17	10.486	1422	1428	1430	rBV	34021	40563	1.59%	0.222%
18	10.616	1446	1450	1462	rBV	1294423	1132996	44.34%	6.188%
19	10.751	1468	1473	1476	rBV2	53767	81713	3.20%	0.446%
20	11.186	1544	1547	1549	rBV	36336	29779	1.17%	0.163%
21	11.216	1549	1552	1557	rVB2	41022	44119	1.73%	0.241%
22	11.316	1565	1569	1573	rBV	840285	688996	26.96%	3.763%
23	11.616	1617	1620	1623	rBV	35890	32202	1.26%	0.176%
24	11.857	1657	1661	1669	rBV	449715	431780	16.90%	2.358%
25	12.027	1687	1690	1693	rVB3	36267	31113	1.22%	0.170%
26	12.410	1751	1755	1757	rBV3	59027	77307	3.03%	0.422%
27	12.645	1792	1795	1801	rBV	195493	204423	8.00%	1.116%
28	12.769	1813	1816	1818	rBV2	39761	47835	1.87%	0.261%
29	12.792	1818	1820	1823	rVB2	39550	34253	1.34%	0.187%
30	12.916	1836	1841	1844	rBV	2596076	2202978	86.21%	12.032%
31	13.151	1878	1881	1884	rBV2	53975	54850	2.15%	0.300%
32	13.357	1914	1916	1919	rVB3	42146	37722	1.48%	0.206%
33	13.827	1994	1996	1998	rBV3	48226	38319	1.50%	0.209%
34	13.969	2017	2020	2024	rBV	708875	671801	26.29%	3.669%
35	15.457	2269	2273	2278	rVB	394287	502311	19.66%	2.743%
36	16.174	2392	2395	2407	rVB3	188090	360400	14.10%	1.968%

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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-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.621	2467	2471	2480	rVB2	168036	311670	12.20%	1.702%
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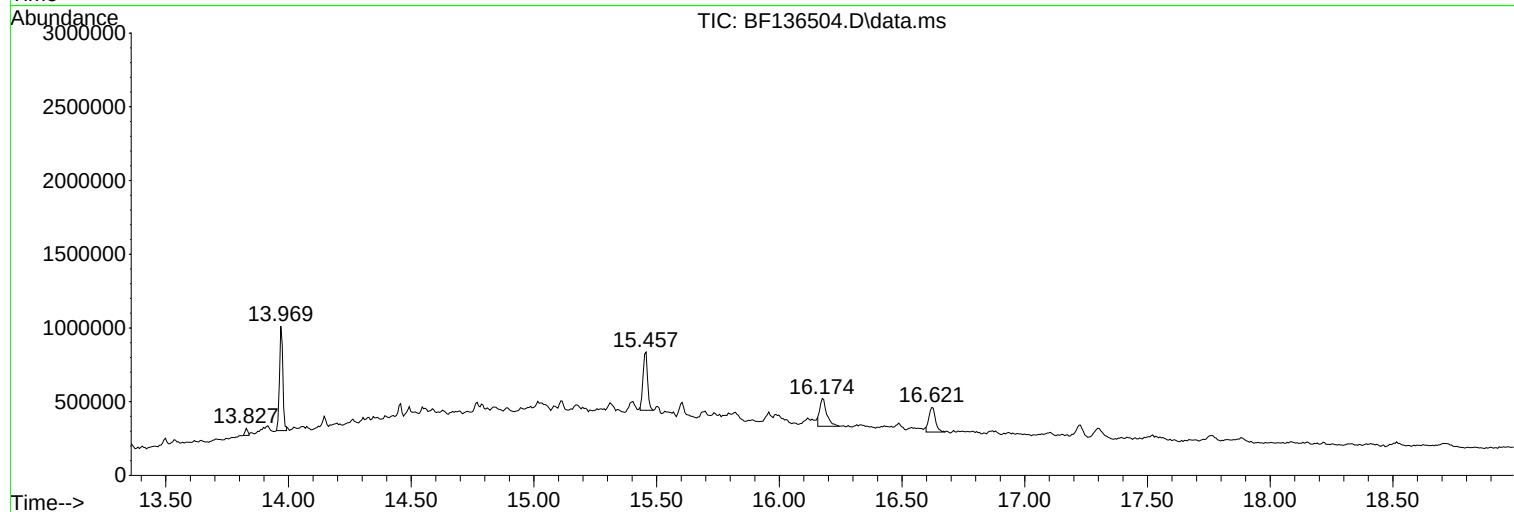
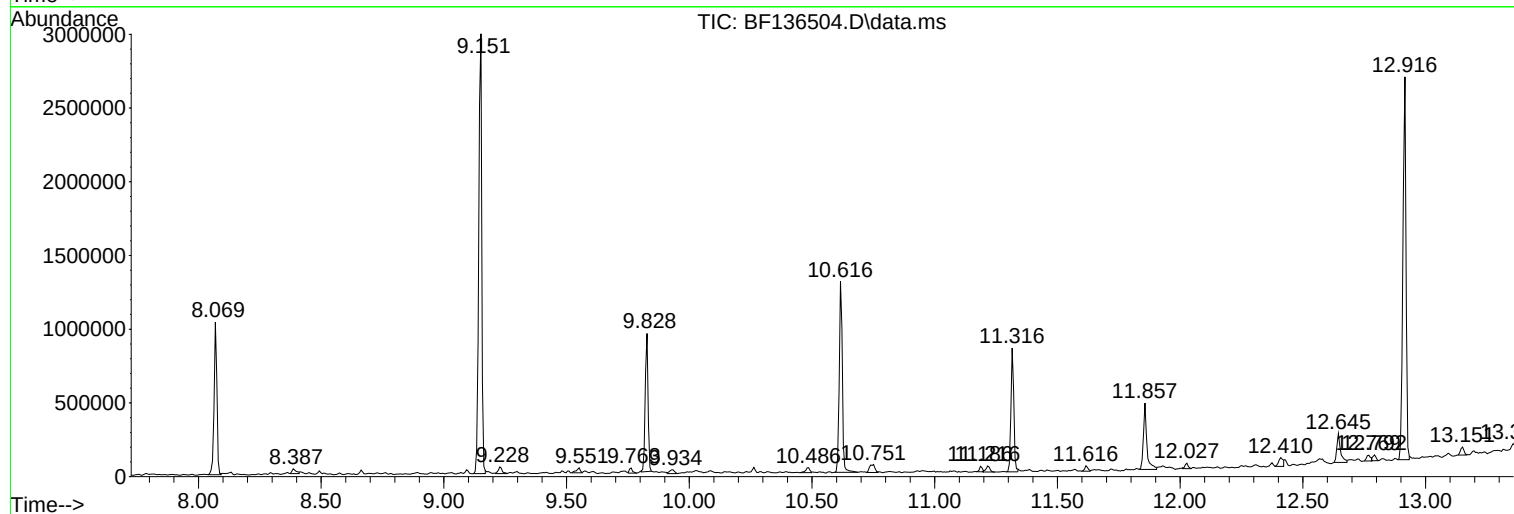
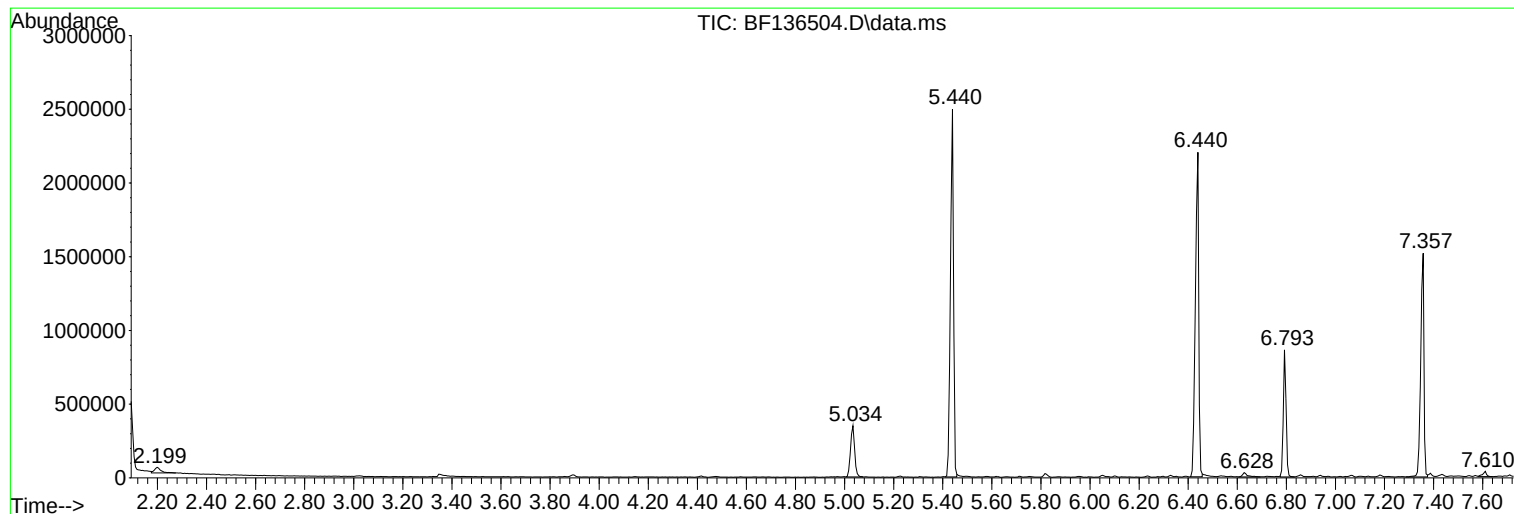
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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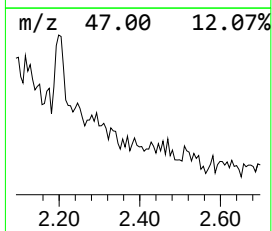
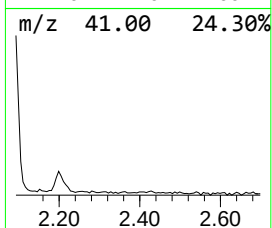
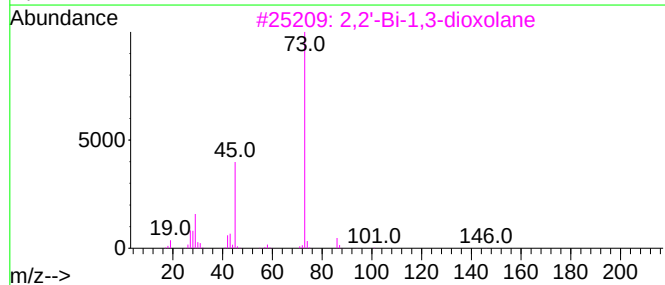
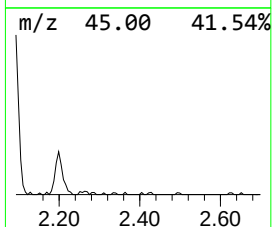
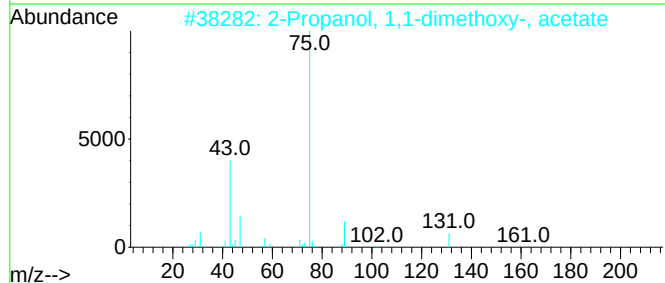
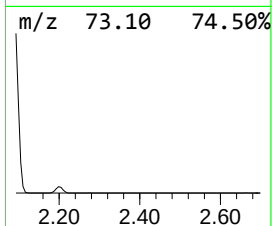
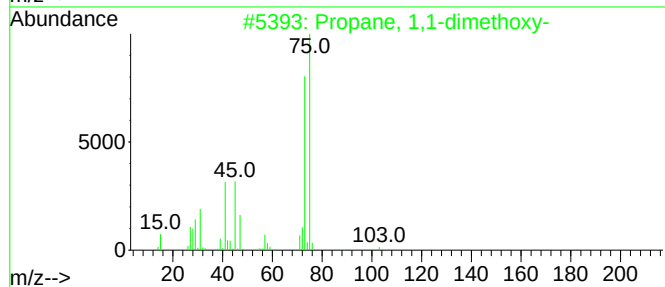
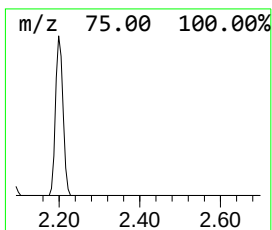
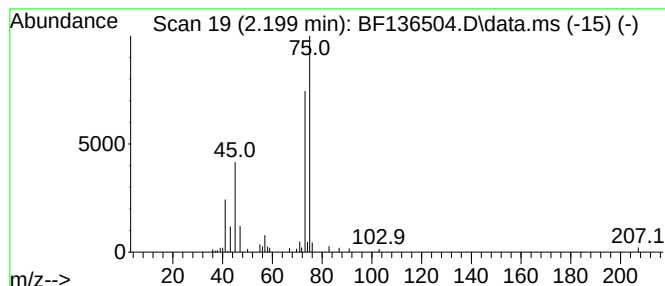
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	2.14 ng	71165	1,4-Dichlorobenzene-d4	6.793

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	50
2		2-Propanol, 1,1-dimethoxy-, acetate	162	C7H14O4	074495-37-7	38
3		2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	16
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
5		2,5-Diethoxy-3-methyl-3-vinylhexane	214	C13H26O2	1000432-70-8	12



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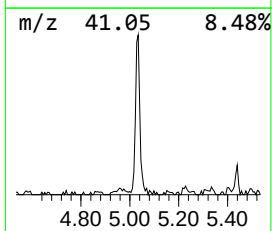
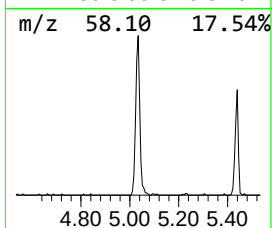
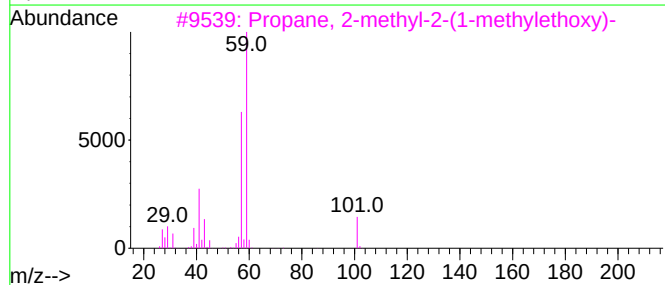
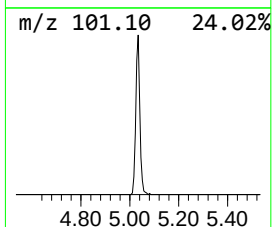
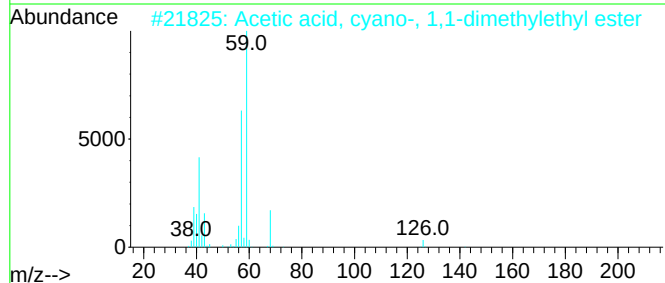
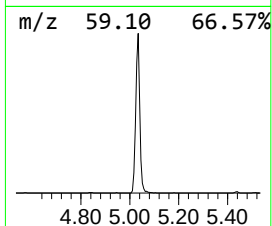
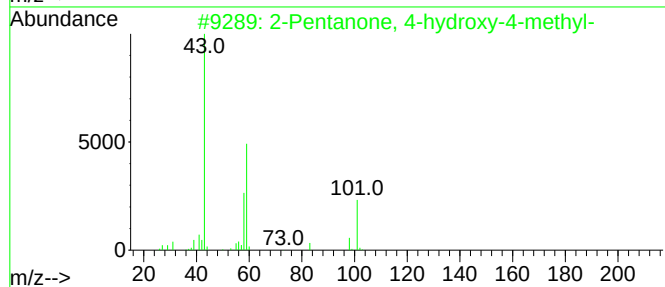
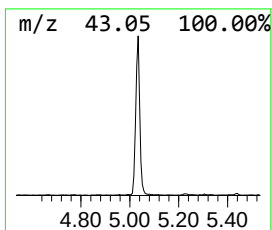
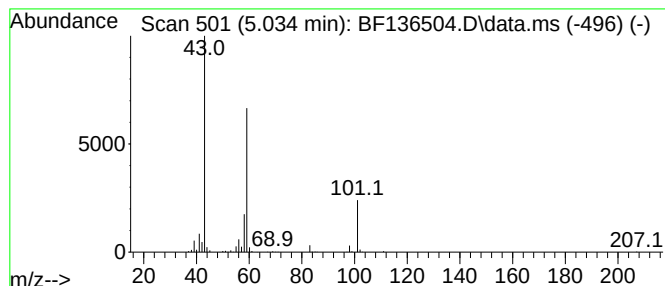
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.034	12.23 ng	406430	1,4-Dichlorobenzene-d4	6.793	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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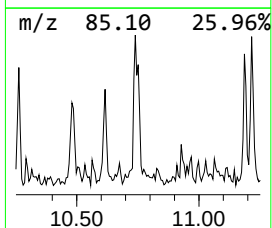
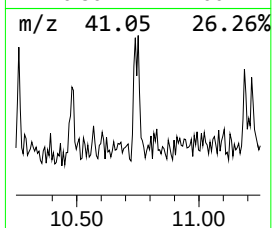
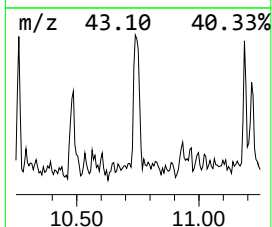
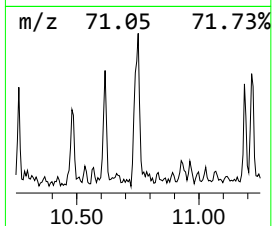
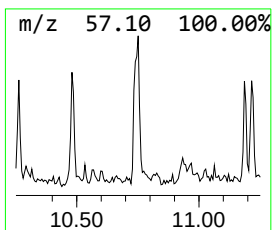
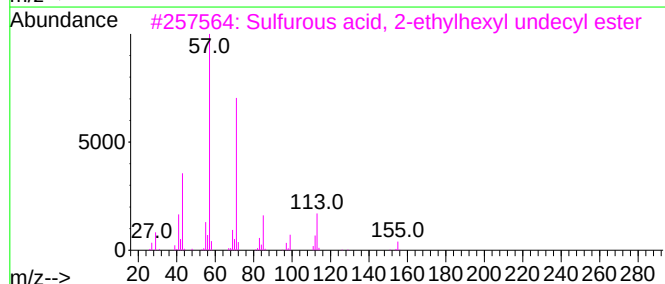
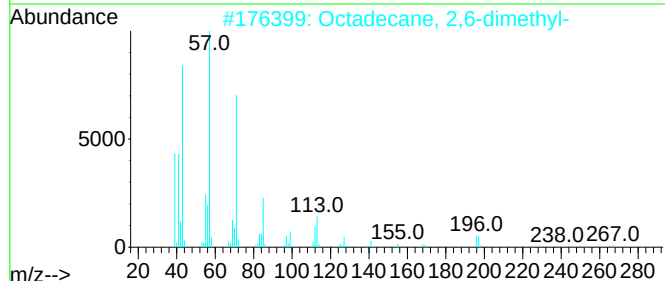
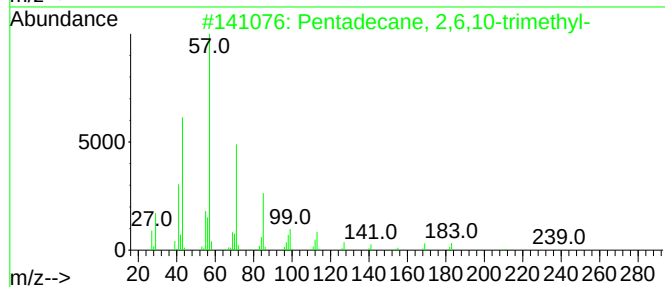
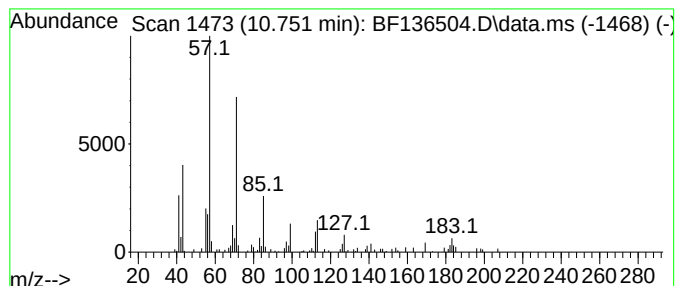
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Pentadecane, 2,6,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.751	2.37 ng	81713	Phenanthrene-d10	11.316	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	86
2	Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	78
3	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	72
4	Heptacosane	380	C27H56	000593-49-7	72
5	Tridecane, 3-methyl-	198	C14H30	006418-41-3	64



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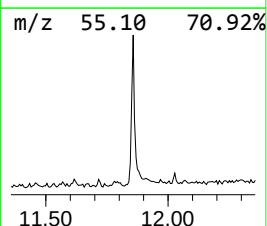
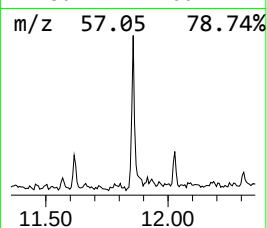
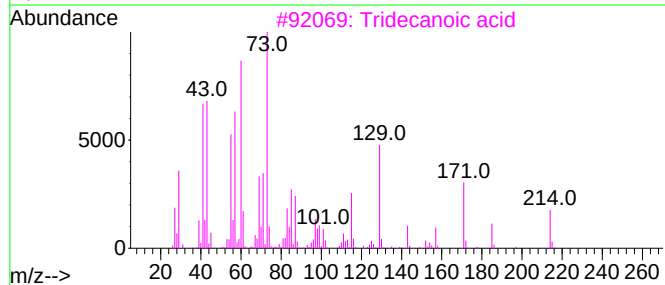
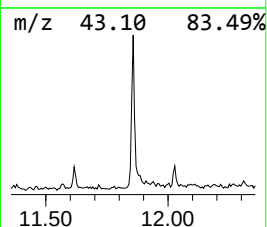
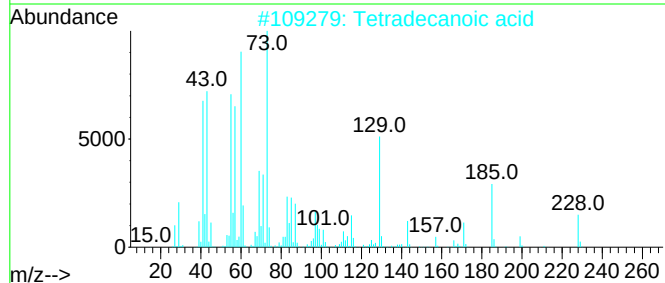
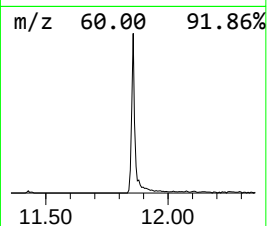
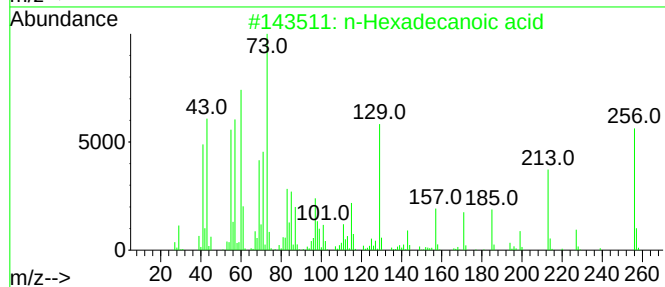
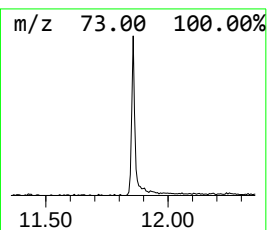
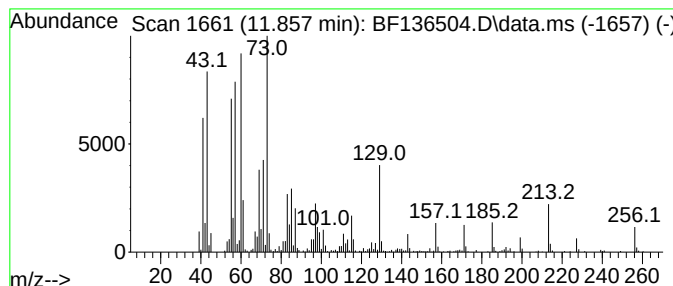
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	12.53 ng	431780	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	96
3			Tridecanoic acid	214	C13H26O2	000638-53-9	94
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			Undecanoic acid	186	C11H22O2	000112-37-8	81



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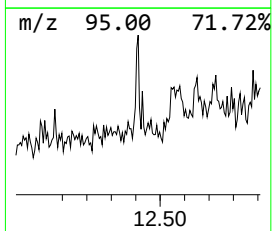
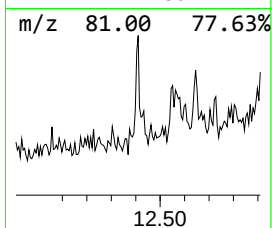
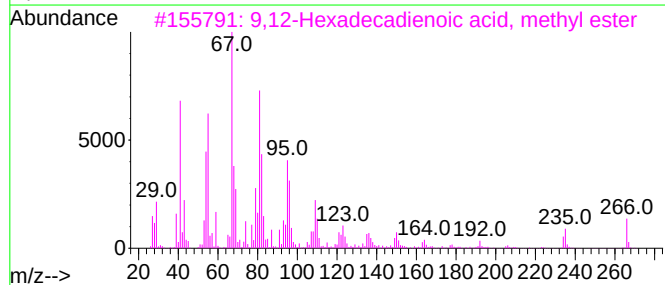
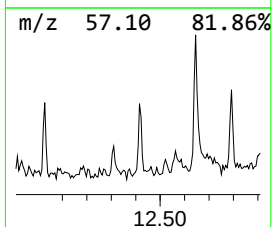
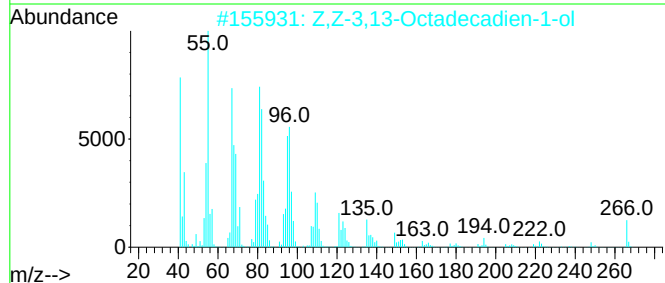
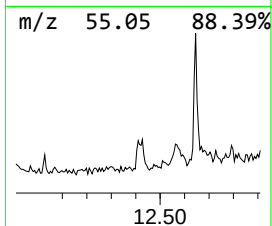
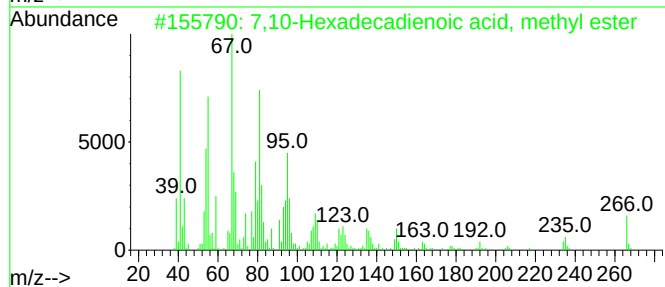
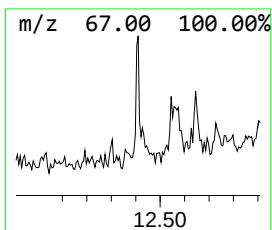
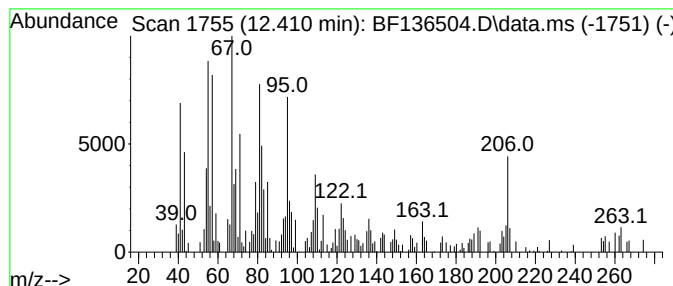
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 7,10-Hexadecadienoic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.410	2.24 ng	77307	Phenanthrene-d10	11.316	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,10-Hexadecadienoic acid, methy...	266	C17H30O2	016106-03-9	83
2	Z,Z-3,13-Octadecadien-1-ol	266	C18H34O	1000131-10-9	64
3	9,12-Hexadecadienoic acid, methy...	266	C17H30O2	002462-80-8	64
4	Oxacycloheptadec-8-en-2-one, (8Z)-	252	C16H28O2	000123-69-3	58
5	(1S,4aS,4bS,7S,8aS,10aS)-7-Isopr...	262	C19H34	002221-95-6	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
Data File : BF136504.D
Acq On : 11 Dec 2023 22:28
Operator : CG\JU
Sample : 05659-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-120623

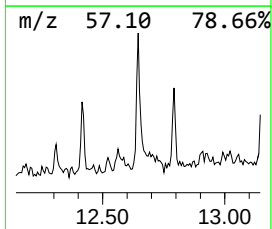
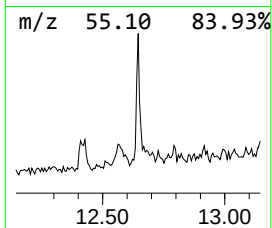
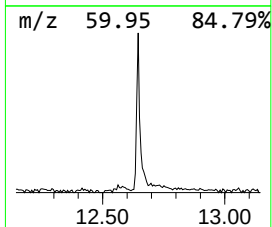
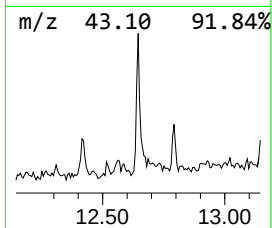
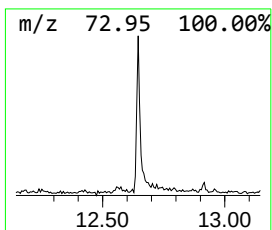
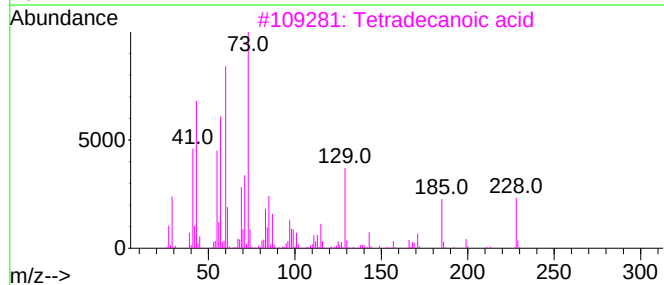
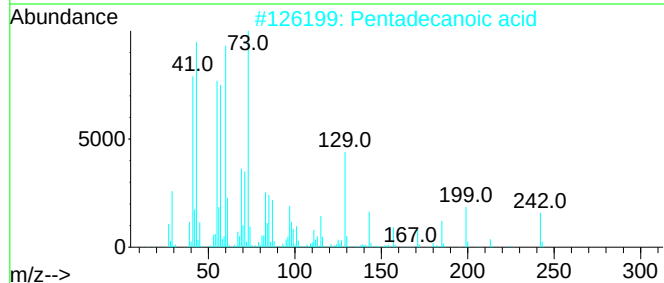
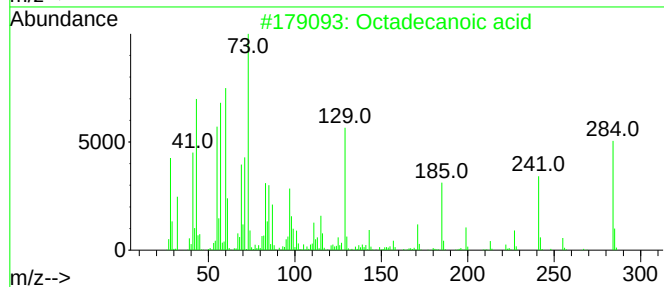
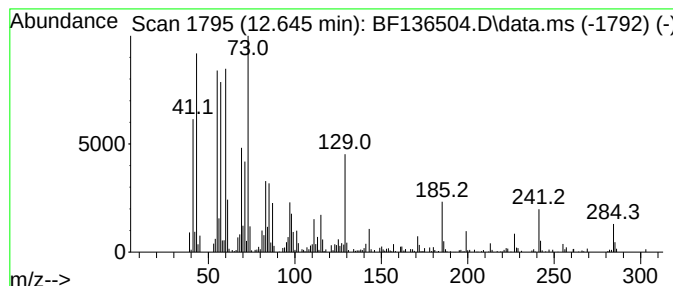
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	6.09 ng	204423	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
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Acq On : 11 Dec 2023 22:28
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Sample : 05659-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-120623

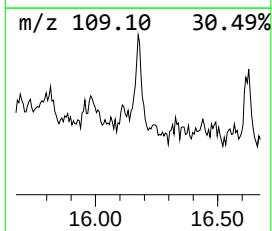
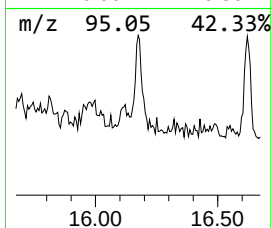
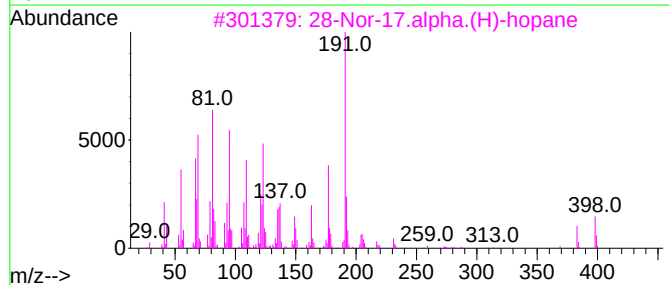
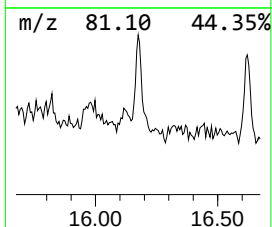
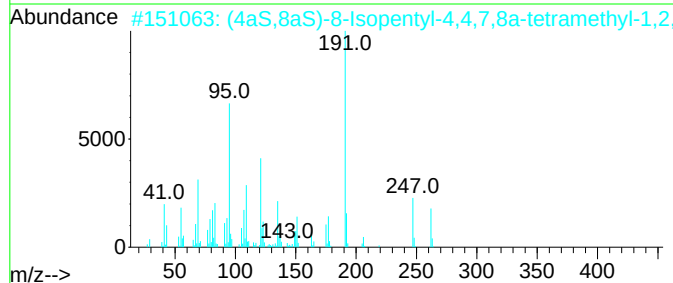
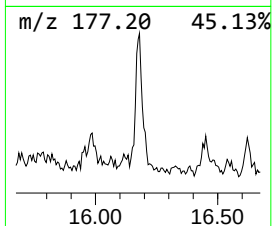
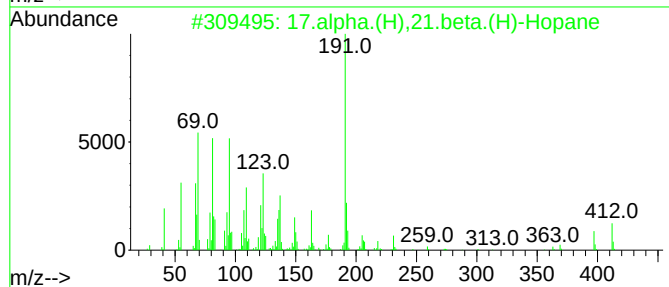
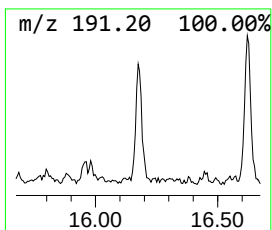
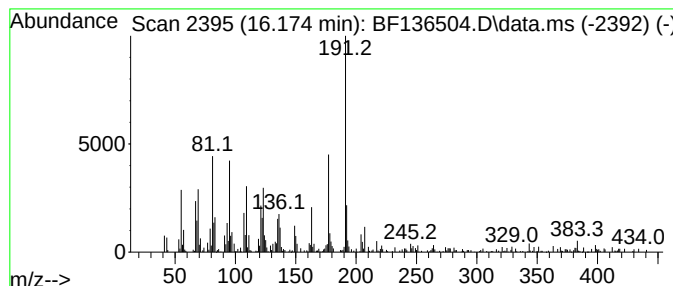
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.174	14.35 ng	360400	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	90
2			(4aS,8aS)-8-Isopentyl-4,4,7,8a-t...	262	C19H34	220766-79-0	64
3			28-Nor-17.alpha.(H)-hopane	398	C29H50	053584-60-4	60
4			28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	52
5			6-(2-Fluoro-phenyl)-5-nitro-pipe...	238	C11H11FN2O3	1000275-16-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-120623

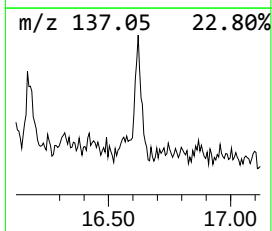
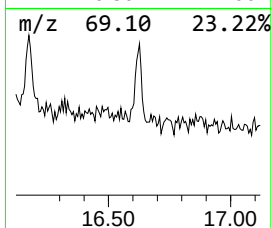
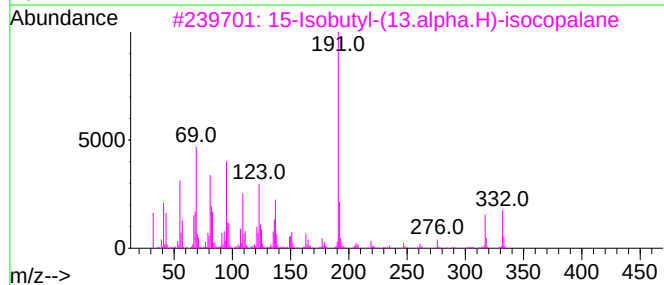
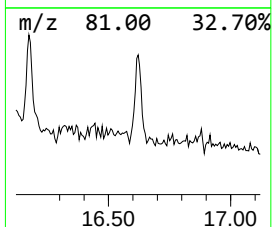
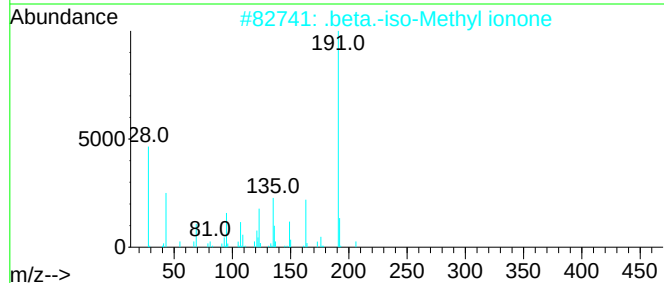
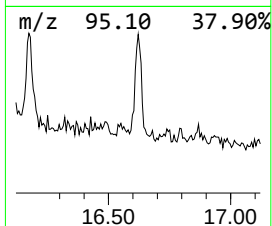
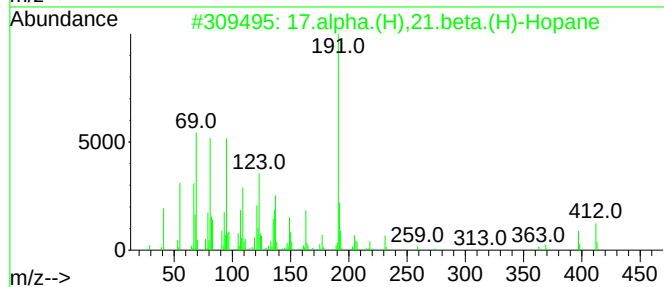
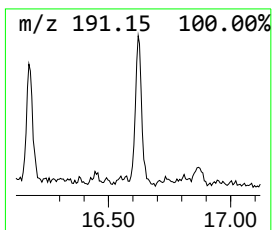
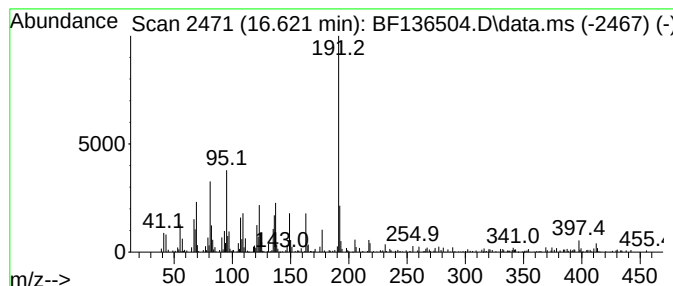
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.621 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.621	12.41 ng	311670	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	91
2			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	49
3			15-Isobutyl-(13.alpha.H)-isocopa...	332	C24H44	087953-47-7	43
4			2-Fluoro-6-trifluoromethylbenzoi...	404	C22H32F4O2	1000338-53-9	38
5			Isophthalic acid, 2-fluorophenyl...	302	C17H15F4O4	1000344-65-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121123\
Data File : BF136504.D
Acq On : 11 Dec 2023 22:28
Operator : CG\JU
Sample : 05659-01
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-04-120623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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
Propane, 1,1-di...	2.199	2.1	ng	71165	1	6.793	664531	20.0
2-Pentanone, 4-...	5.034	12.2	ng	406430	1	6.793	664531	20.0
Pentadecane, 2,...	10.751	2.4	ng	81713	4	11.316	688996	20.0
n-Hexadecanoic ...	11.857	12.5	ng	431780	4	11.316	688996	20.0
7,10-Hexadecadi...	12.410	2.2	ng	77307	4	11.316	688996	20.0
Octadecanoic acid	12.645	6.1	ng	204423	5	13.969	671801	20.0
17.alpha.(H),21...	16.174	14.4	ng	360400	6	15.457	502311	20.0
unknown16.621	16.621	12.4	ng	311670	6	15.457	502311	20.0