

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112921\
 Data File : BP008139.D
 Acq On : 29 Nov 2021 13:42
 Operator : CG/JU
 Sample : M4843-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 L-1

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_P\Methods\8270E-BP112521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008139.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.052	9	11	31	rVB3	61973	122581	3.00%	0.555%
2	4.928	325	330	342	rVB	147596	212034	5.19%	0.960%
3	5.393	402	409	426	rBV	1304901	1978580	48.41%	8.954%
4	6.981	670	679	695	rBV	1198925	2077479	50.83%	9.401%
5	7.805	812	819	827	rBV	296815	474303	11.60%	2.146%
6	8.963	1008	1016	1030	rBV	777447	1314028	32.15%	5.947%
7	10.399	1251	1260	1268	rBV	26962	57947	1.42%	0.262%
8	10.599	1286	1294	1302	rBV	369992	627621	15.36%	2.840%
9	13.069	1707	1714	1722	rBV	1834251	2654063	64.94%	12.011%
10	14.104	1885	1890	1899	rBV3	25099	48204	1.18%	0.218%
11	14.446	1940	1948	1957	rBV	551107	828490	20.27%	3.749%
12	15.275	2082	2089	2094	rBV2	38329	84949	2.08%	0.384%
13	15.945	2196	2203	2211	rBV	1510220	2195427	53.72%	9.935%
14	16.781	2340	2345	2352	rBV	29210	50365	1.23%	0.228%
15	17.139	2402	2406	2410	rVB	41538	49016	1.20%	0.222%
16	17.204	2411	2417	2422	rBV	700792	1026600	25.12%	4.646%
17	17.328	2436	2438	2444	rVB5	27742	43681	1.07%	0.198%
18	18.104	2566	2570	2578	rBV	149424	208937	5.11%	0.946%
19	18.175	2578	2582	2586	rVB	44340	56297	1.38%	0.255%
20	19.222	2756	2760	2770	rBV	107768	167464	4.10%	0.758%
21	19.345	2777	2781	2784	rBV2	59573	86919	2.13%	0.393%
22	19.575	2817	2820	2830	rVB	81934	130482	3.19%	0.590%
23	19.775	2849	2854	2860	rBV	3155882	4087165	100.00%	18.496%
24	20.528	2978	2982	2987	rBV	176598	220534	5.40%	0.998%
25	20.869	3037	3040	3043	rBV	51444	57231	1.40%	0.259%
26	21.028	3063	3067	3074	rVV2	302430	425489	10.41%	1.926%
27	21.086	3075	3077	3084	rVB2	56319	63831	1.56%	0.289%
28	21.304	3109	3114	3119	rBV	1004412	1384903	33.88%	6.267%
29	23.698	3515	3521	3532	rVB2	679059	1362761	33.34%	6.167%

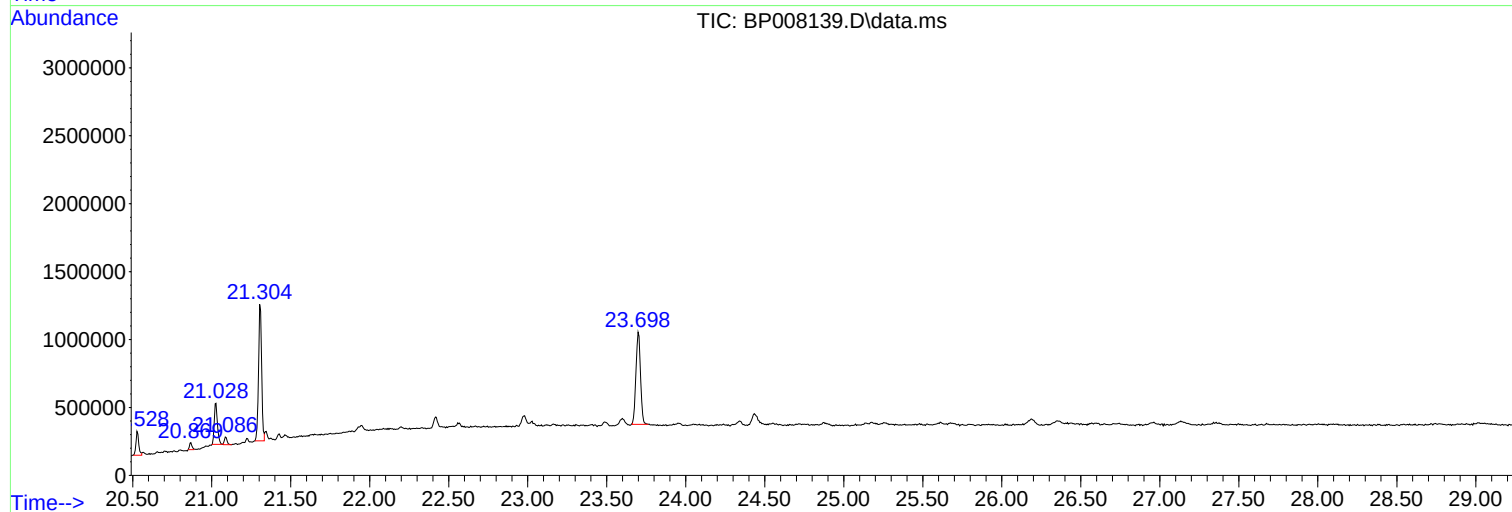
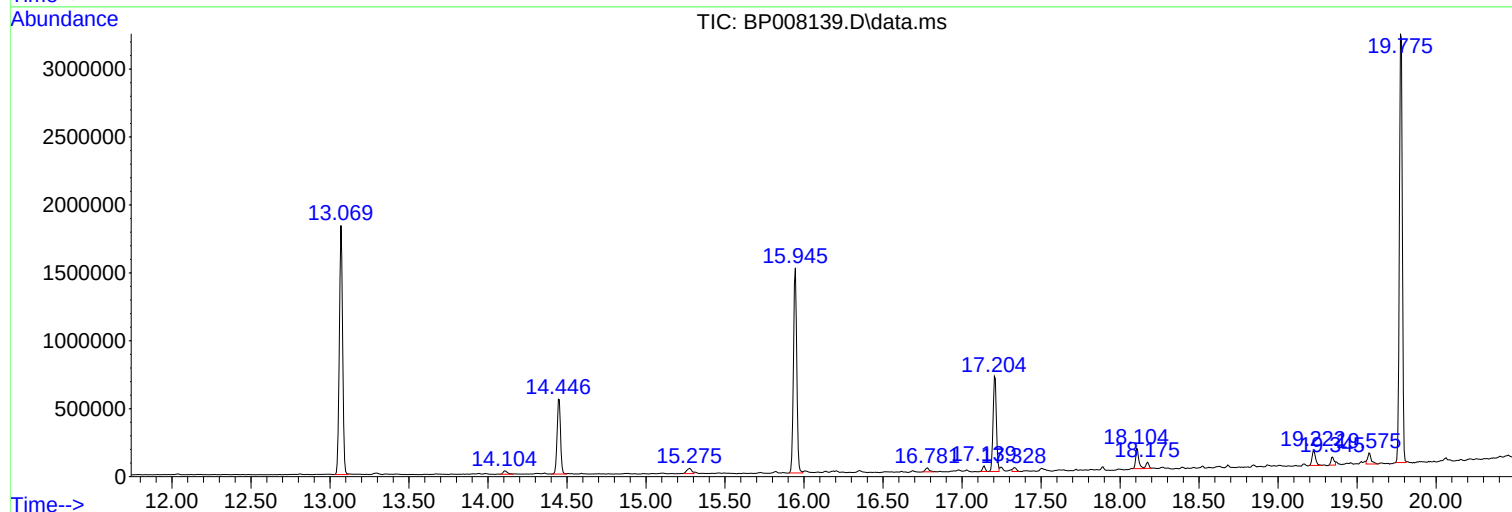
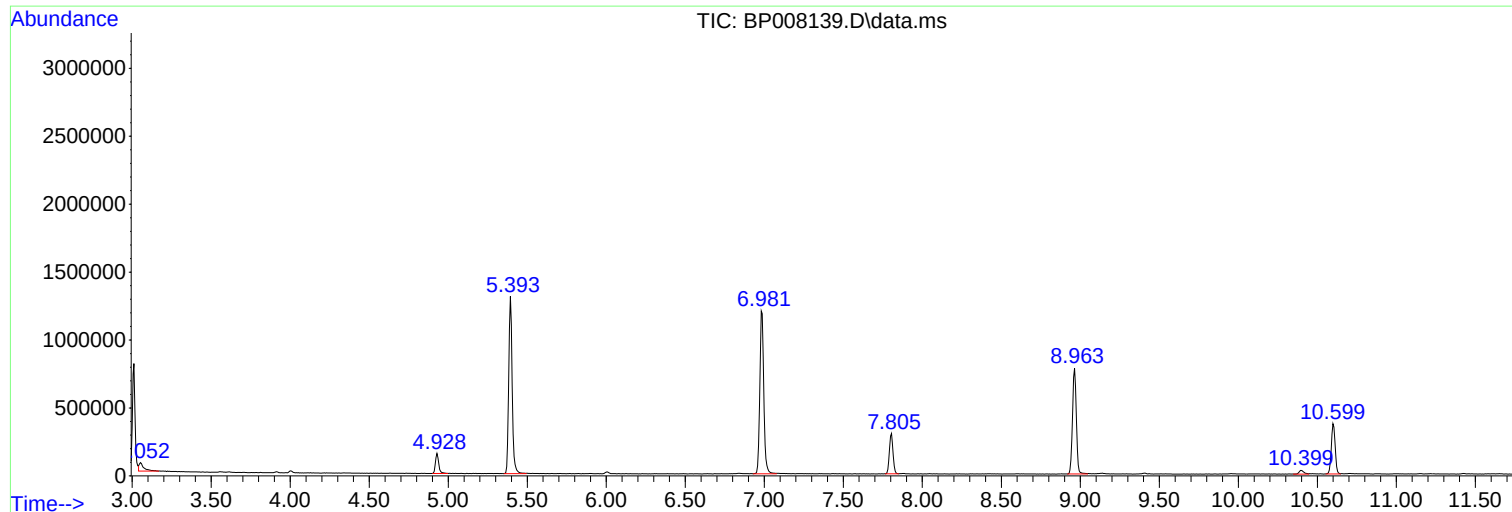
Sum of corrected areas: 22097381

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112921\
Data File : BP008139.D
Acq On : 29 Nov 2021 13:42
Operator : CG/JU
Sample : M4843-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
L-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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_P\Data\BP112921\
Data File : BP008139.D
Acq On : 29 Nov 2021 13:42
Operator : CG/JU
Sample : M4843-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
L-1

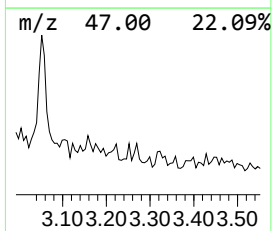
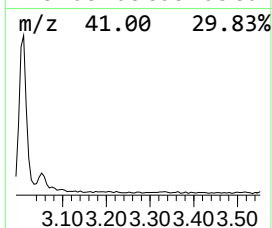
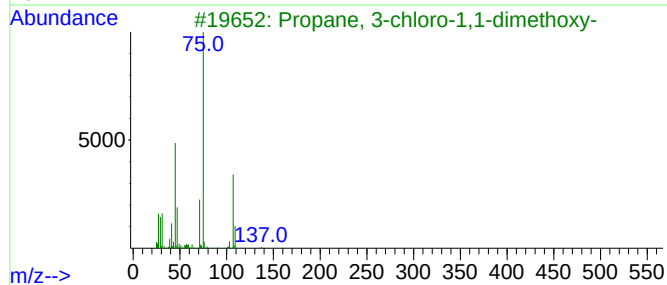
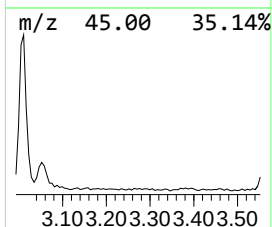
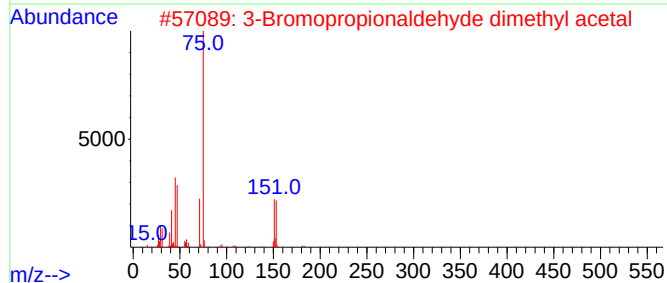
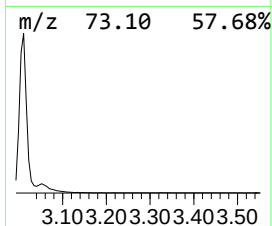
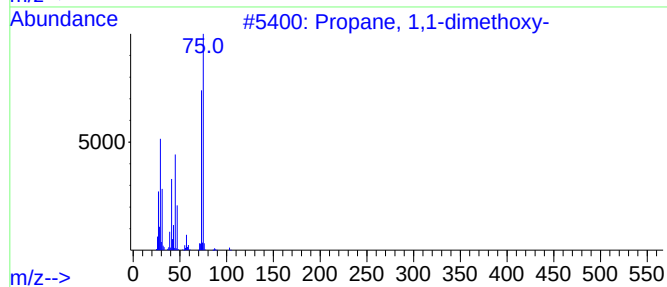
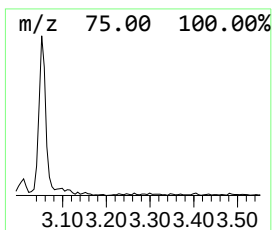
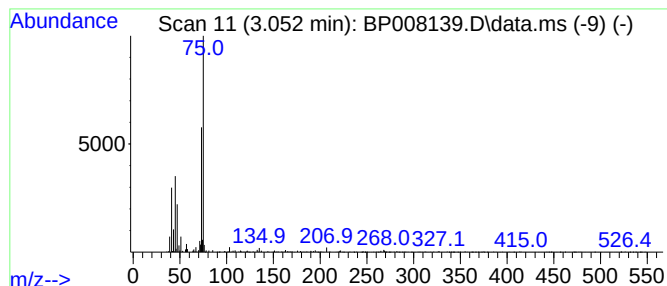
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.052	5.17 ng	122581	1,4-Dichlorobenzene-d4	7.805

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	50
3			Propane, 3-chloro-1,1-dimethoxy-	138	C5H11ClO2	035502-06-8	38
4			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	38
5			4-Methylvaleric acid, TMS deriva...	188	C9H20O2Si	959048-10-3	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112921\
Data File : BP008139.D
Acq On : 29 Nov 2021 13:42
Operator : CG/JU
Sample : M4843-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

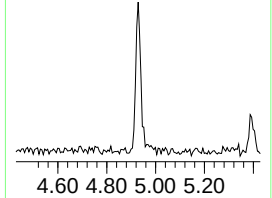
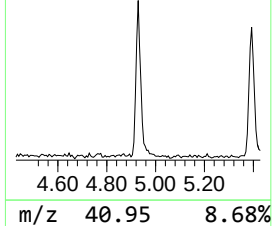
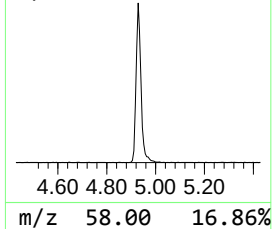
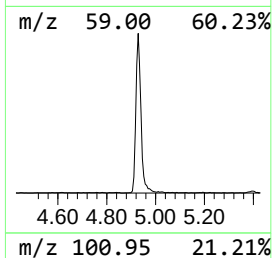
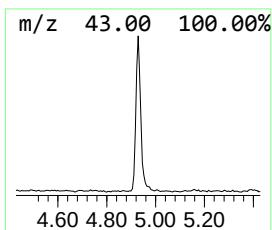
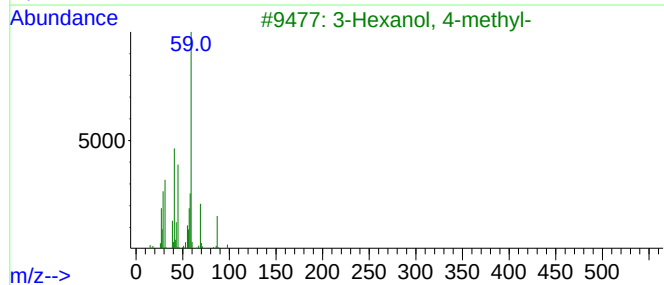
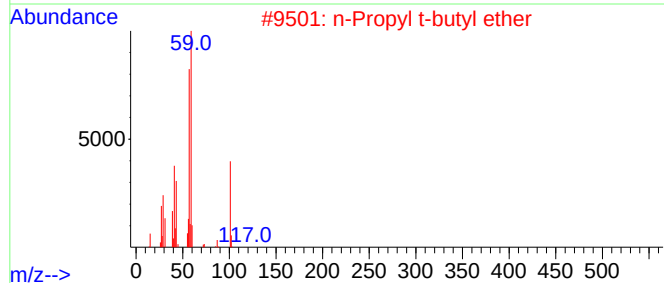
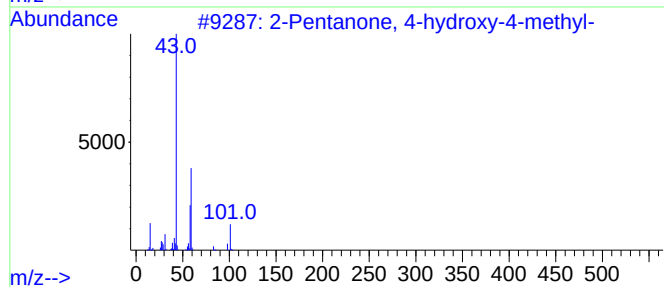
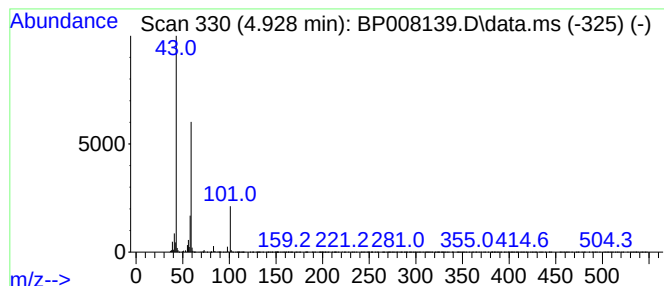
Instrument :
BNA_P
ClientSampleId :
L-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.928	8.94 ng	212034	1,4-Dichlorobenzene-d4			7.805
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	72
2	n-Propyl t-butyl ether		116	C7H16O	1000334-81-9	33
3	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	28
4	2,5,8,11-Tetraoxadodecane		178	C8H18O4	000112-49-2	23
5	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112921\
Data File : BP008139.D
Acq On : 29 Nov 2021 13:42
Operator : CG/JU
Sample : M4843-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
L-1

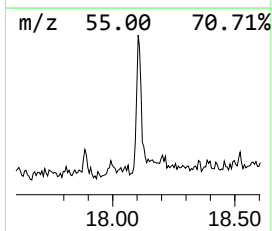
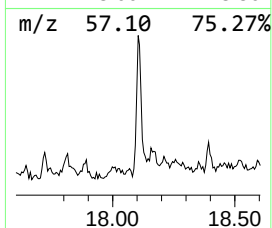
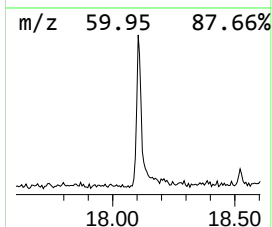
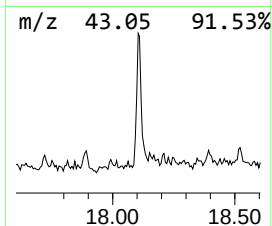
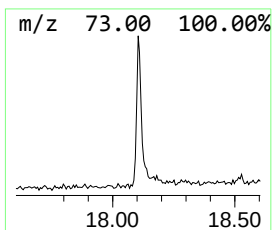
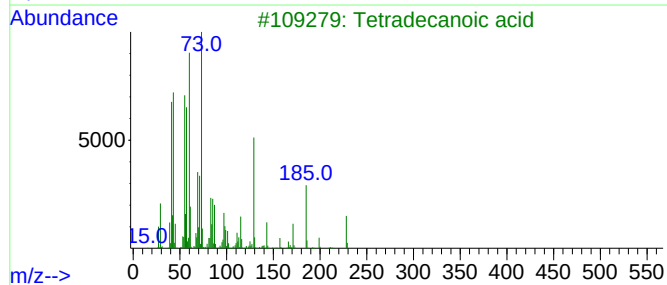
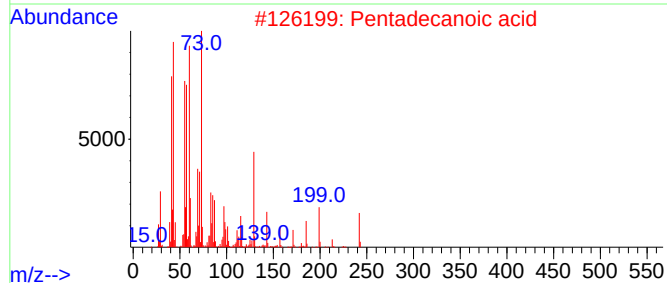
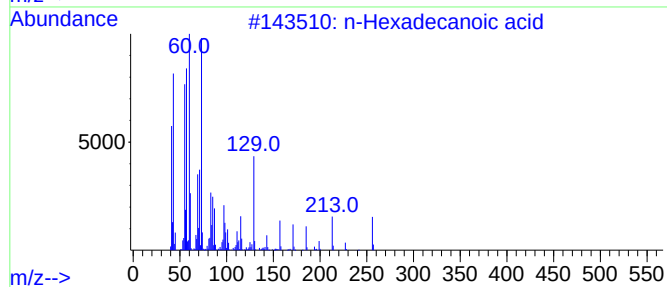
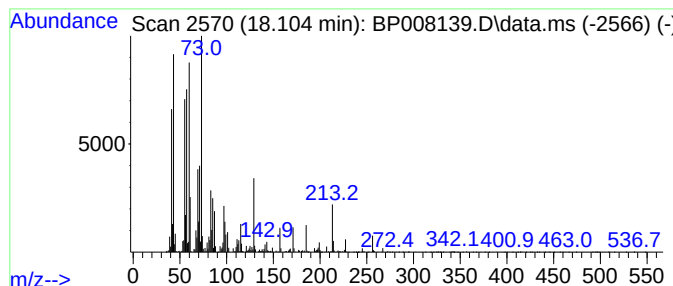
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	4.07 ng	208937	Phenanthrene-d10	17.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112921\
Data File : BP008139.D
Acq On : 29 Nov 2021 13:42
Operator : CG/JU
Sample : M4843-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

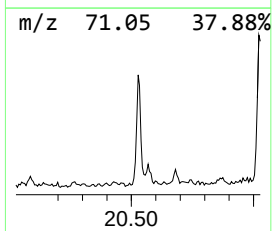
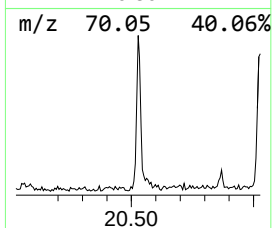
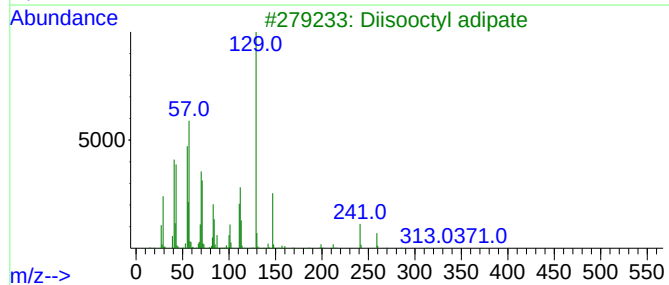
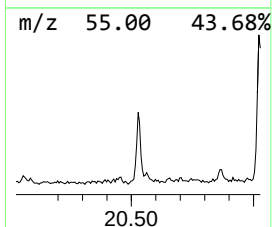
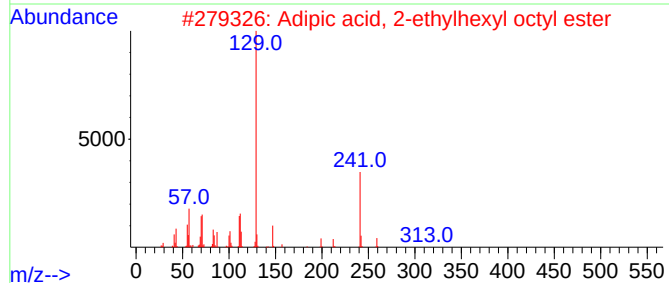
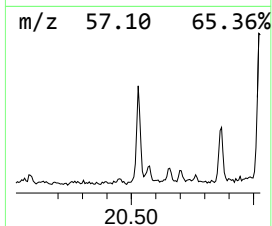
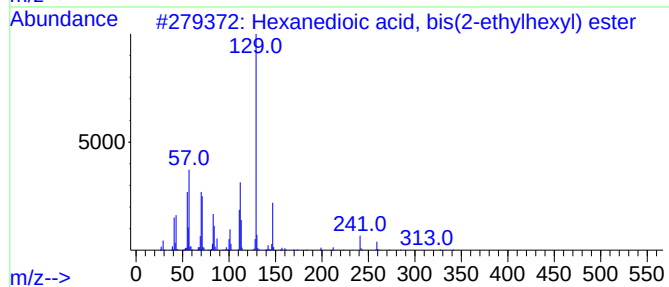
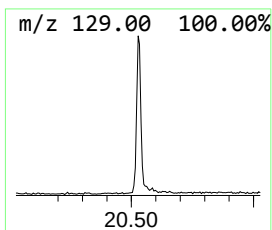
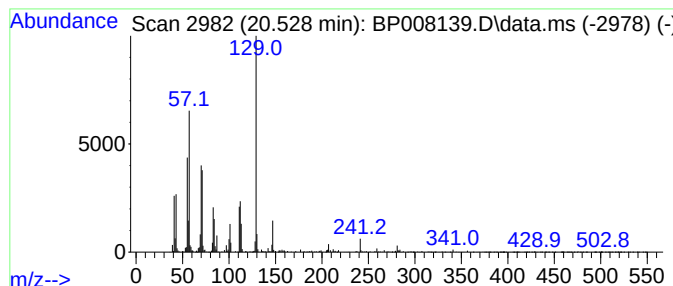
Instrument :
BNA_P
ClientSampleId :
L-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexanedioic acid, bis(2-eth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.528	3.18 ng	220534	Chrysene-d12	21.304	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
2	Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
3	Diisooctyl adipate	370	C22H42O4	001330-86-5	80
4	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	74
5	Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112921\
Data File : BP008139.D
Acq On : 29 Nov 2021 13:42
Operator : CG/JU
Sample : M4843-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
L-1

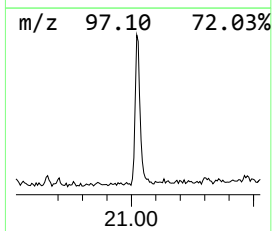
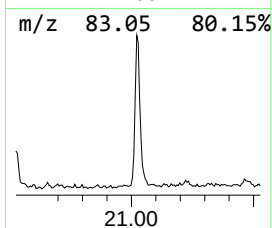
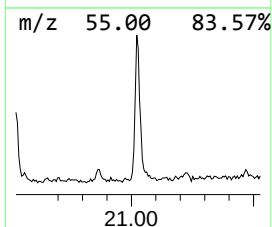
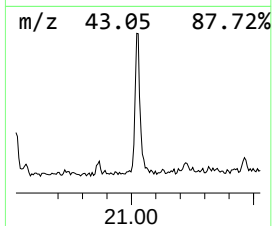
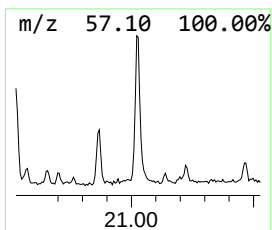
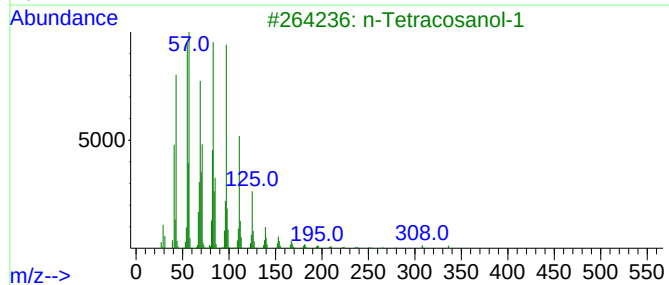
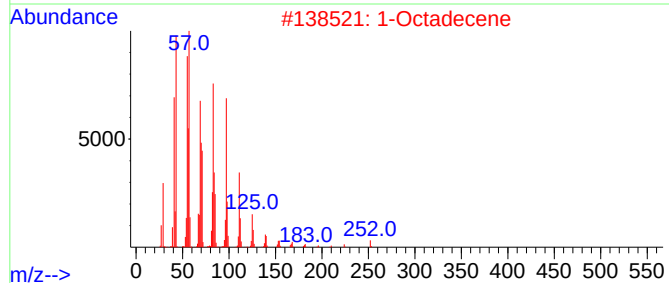
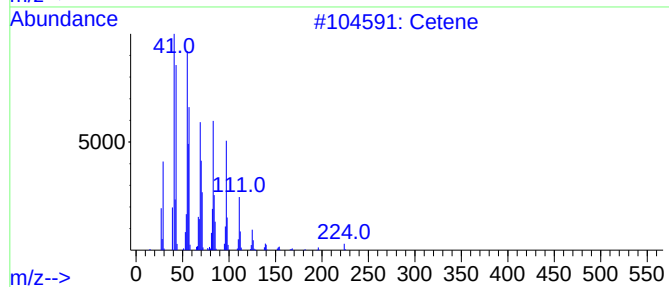
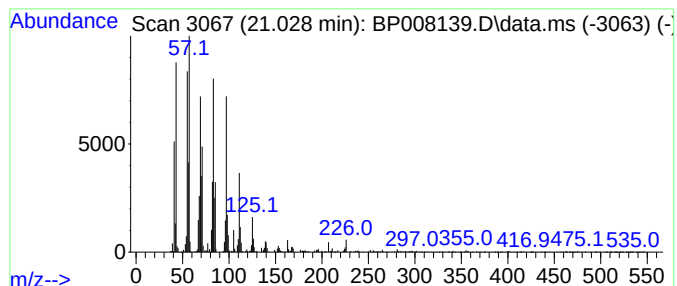
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cetene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.028	6.14 ng	425489	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene			224	C16H32	000629-73-2	96
2	1-Octadecene			252	C18H36	000112-88-9	96
3	n-Tetracosanol-1			354	C24H50O	000506-51-4	94
4	Behenic alcohol			326	C22H46O	000661-19-8	94
5	Dichloroacetic acid, heptadecyl ...			366	C19H36Cl2O2	1000282-98-2	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112921\
Data File : BP008139.D
Acq On : 29 Nov 2021 13:42
Operator : CG/JU
Sample : M4843-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
L-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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
Propane, 1,1-di...	3.052	5.2	ng	122581	1	7.805	474303	20.0
2-Pentanone, 4-...	4.928	8.9	ng	212034	1	7.805	474303	20.0
n-Hexadecanoic ...	18.104	4.1	ng	208937	4	17.204	1026600	20.0
Hexanedioic aci...	20.528	3.2	ng	220534	5	21.304	1384900	20.0
Cetene	21.028	6.1	ng	425489	5	21.304	1384900	20.0