

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
 Data File : BF125526.D
 Acq On : 16 Sep 2021 2:59
 Operator : JU/CG
 Sample : M3687-27 5X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A011145

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-BF091521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125526.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	5	9	17	rVB	282260	334551	29.14%	3.144%
2	2.275	30	32	40	rVB	19747	28638	2.49%	0.269%
3	4.393	384	392	400	rVB2	20222	48693	4.24%	0.458%
4	4.587	421	425	430	rVB	25531	30239	2.63%	0.284%
5	5.069	504	507	515	rBV	108586	117187	10.21%	1.101%
6	5.487	574	578	585	rBV	610777	579504	50.47%	5.447%
7	5.616	594	600	604	rBV4	13456	28156	2.45%	0.265%
8	6.298	712	716	719	rVB3	19873	23732	2.07%	0.223%
9	6.498	747	750	759	rBV	582500	683753	59.55%	6.427%
10	6.869	809	813	816	rBV	1048963	952150	82.92%	8.949%
11	7.263	875	880	884	rBV6	13641	23965	2.09%	0.225%
12	7.428	904	908	915	rBV	350574	309880	26.99%	2.913%
13	7.910	984	990	996	rBV	204816	285394	24.86%	2.682%
14	8.069	1013	1017	1018	rBV	28908	35794	3.12%	0.336%
15	8.151	1026	1031	1034	rBV	1387189	1148235	100.00%	10.792%
16	8.181	1034	1036	1046	rVB4	19899	31463	2.74%	0.296%
17	8.510	1088	1092	1104	rBV	298893	356099	31.01%	3.347%
18	8.875	1151	1154	1158	rBV2	16440	24134	2.10%	0.227%
19	9.075	1184	1188	1196	rBV	297782	313683	27.32%	2.948%
20	9.222	1210	1213	1217	rBV	779387	625936	54.51%	5.883%
21	9.333	1229	1232	1237	rBV6	26655	54444	4.74%	0.512%
22	9.375	1237	1239	1244	rVB4	29991	27075	2.36%	0.254%
23	9.604	1276	1278	1282	rBV	111546	130668	11.38%	1.228%
24	9.910	1326	1330	1333	rVB	1186078	1079097	93.98%	10.142%
25	10.363	1405	1407	1411	rBV4	40424	44164	3.85%	0.415%
26	10.698	1460	1464	1469	rBV	286064	288446	25.12%	2.711%
27	11.398	1579	1583	1586	rBV	1122292	942473	82.08%	8.858%
28	11.927	1669	1673	1677	rBV2	605883	648470	56.48%	6.095%
29	12.716	1804	1807	1814	rBV	321301	374964	32.66%	3.524%
30	12.980	1850	1852	1857	rVB	509731	435403	37.92%	4.092%
31	14.051	2031	2034	2037	rVB	719527	633124	55.14%	5.951%

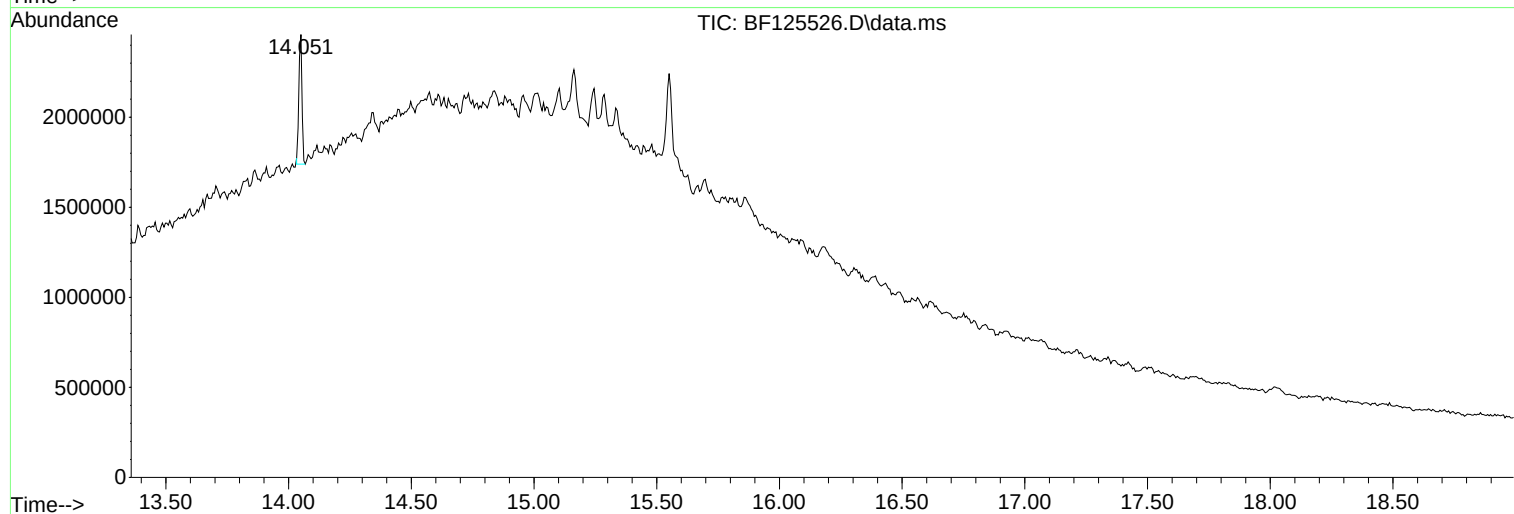
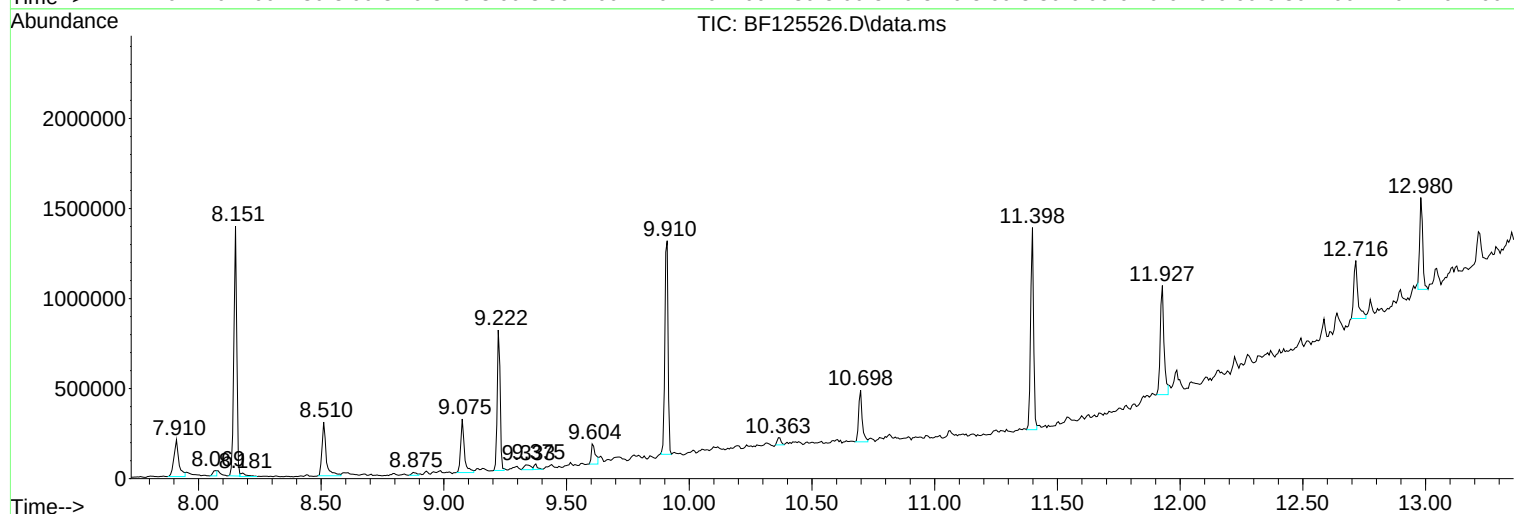
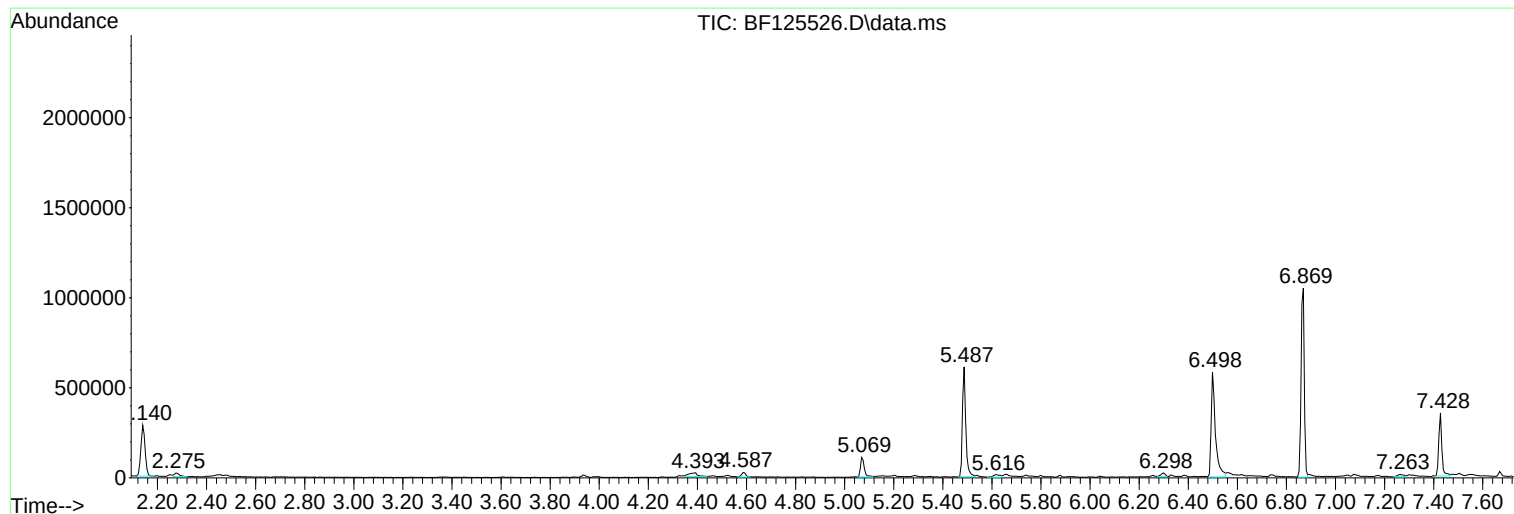
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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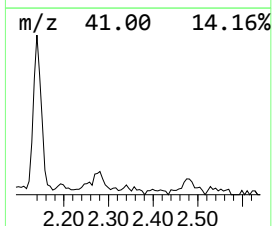
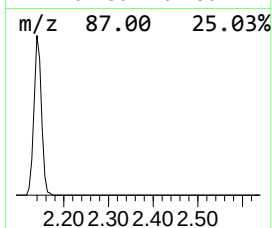
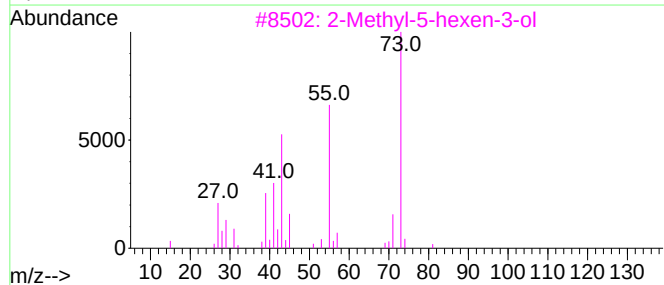
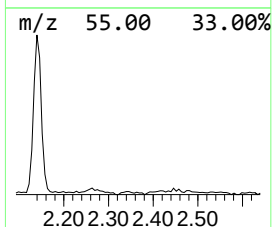
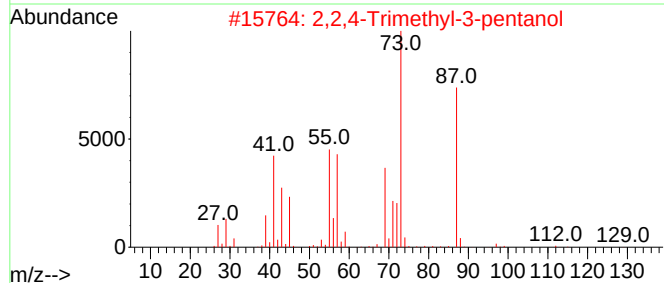
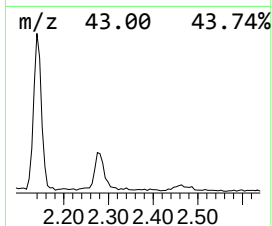
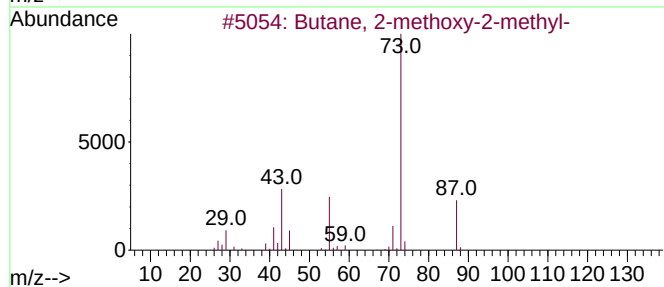
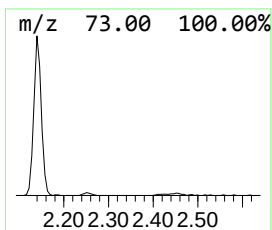
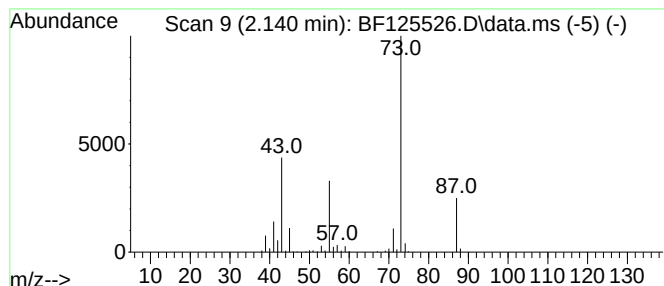
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	7.03 ng	334551	1,4-Dichlorobenzene-d4	6.869

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	40
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	23



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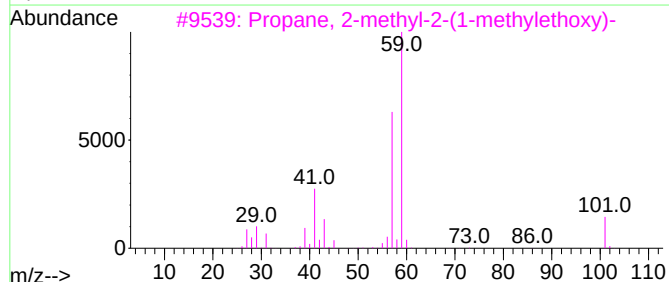
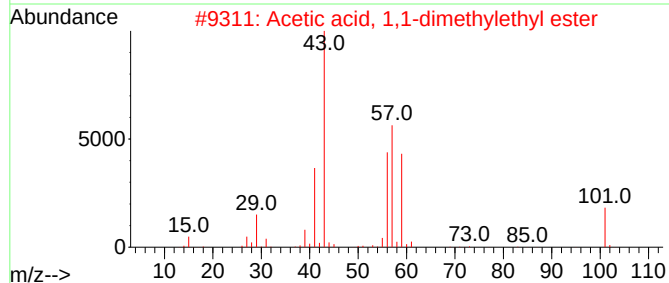
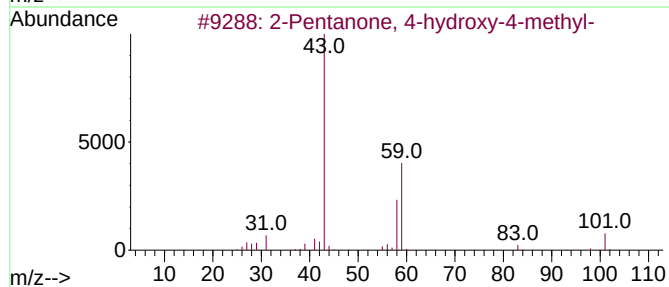
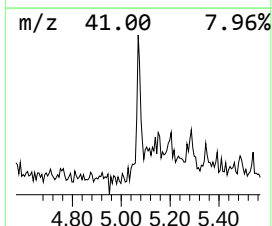
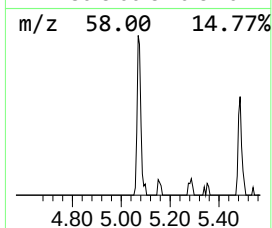
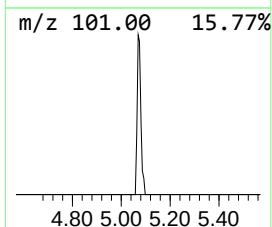
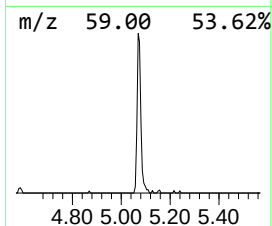
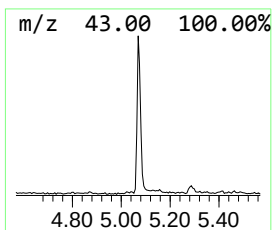
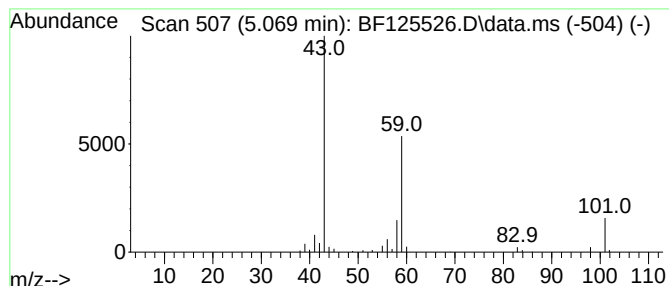
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	2.46 ng	117187	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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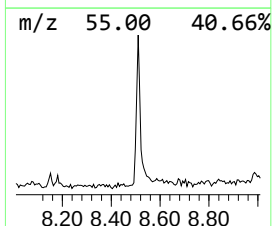
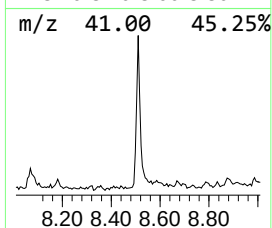
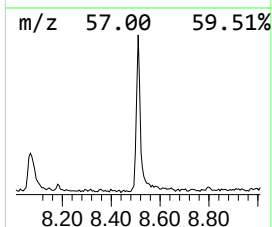
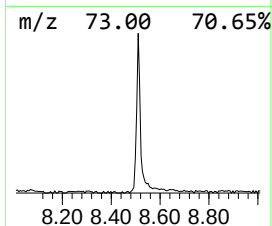
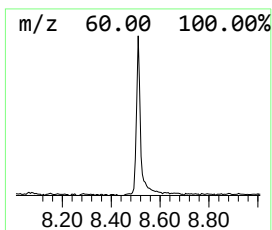
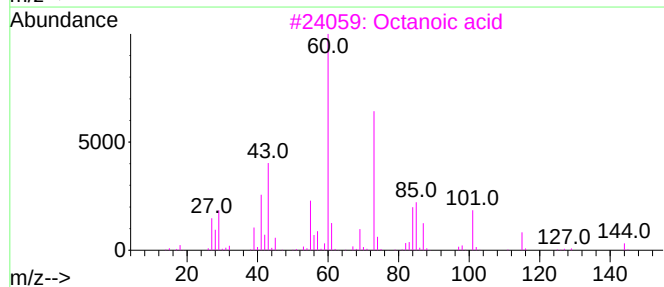
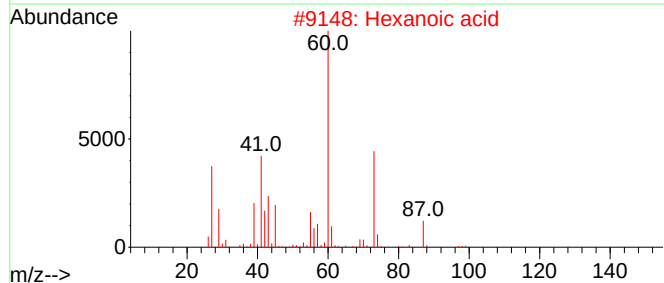
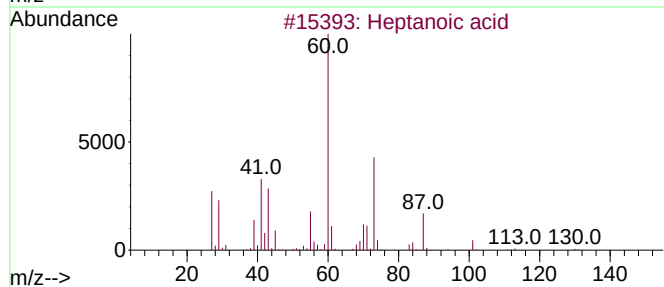
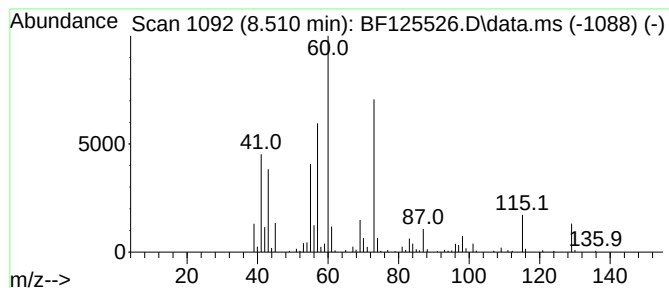
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Peak Number 3 Heptanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.510	6.20 ng	356099	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanoic acid	130	C7H14O2	000111-14-8	72
2			Hexanoic acid	116	C6H12O2	000142-62-1	64
3			Octanoic acid	144	C8H16O2	000124-07-2	59
4			Pentanoic acid	102	C5H10O2	000109-52-4	58
5			Nonanoic acid	158	C9H18O2	000112-05-0	53



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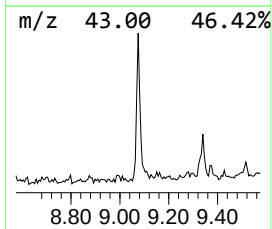
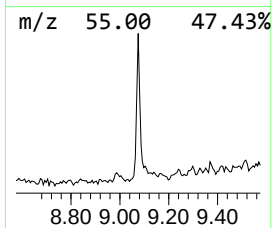
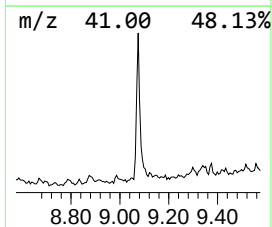
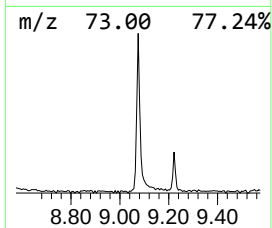
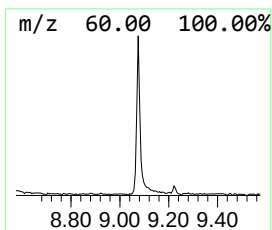
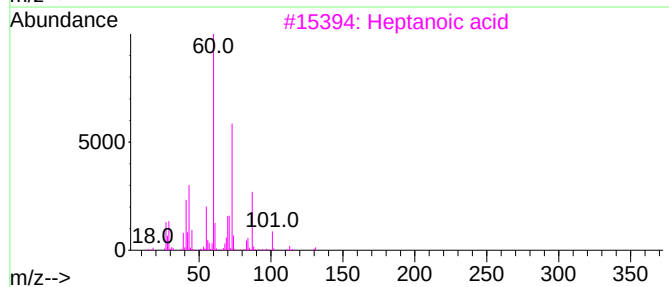
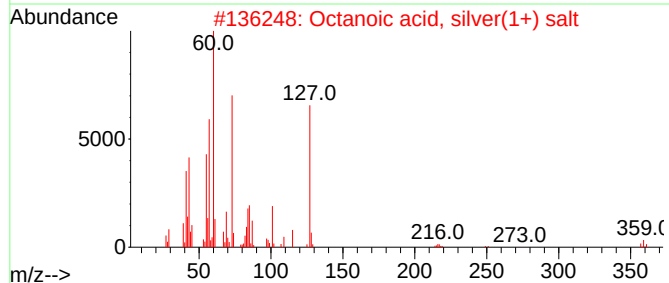
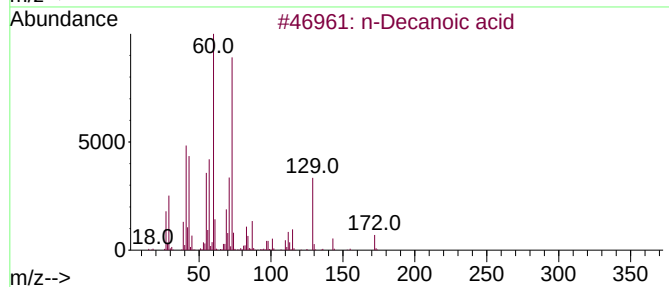
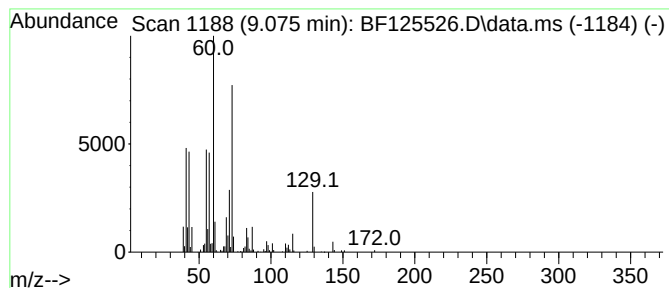
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Decanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.075	5.81 ng	313683	Acenaphthene-d10	9.910

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Decanoic acid	172	C10H20O2	000334-48-5	90
2		Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	58
3		Heptanoic acid	130	C7H14O2	000111-14-8	53
4		Hexanoic acid	116	C6H12O2	000142-62-1	52
5		Octanoic acid	144	C8H16O2	000124-07-2	47



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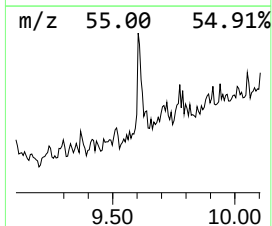
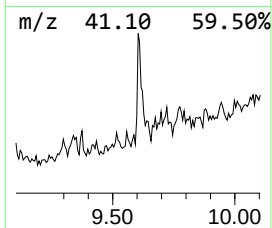
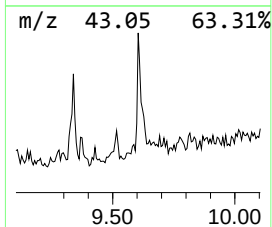
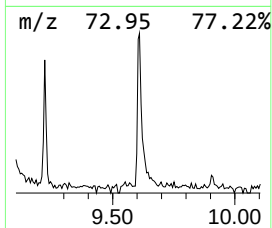
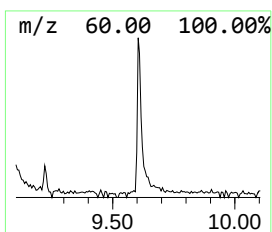
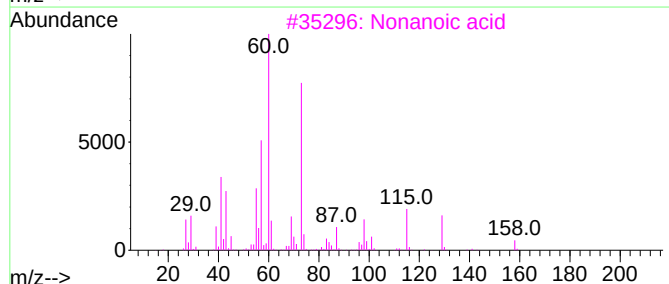
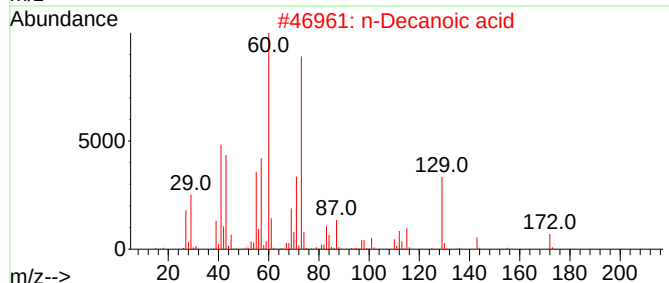
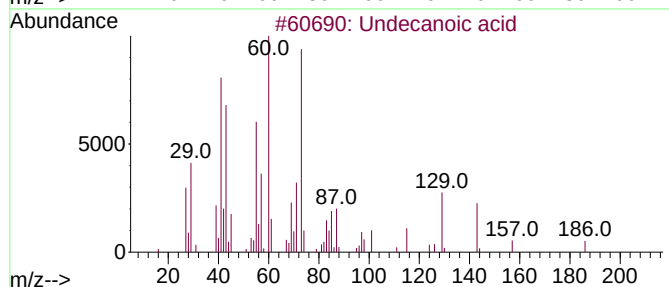
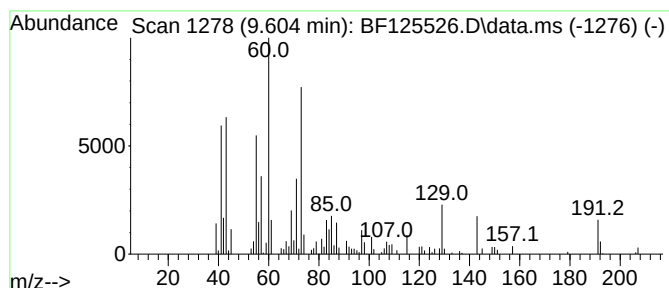
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.604	2.42 ng	130668	Acenaphthene-d10	9.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	87
2			n-Decanoic acid	172	C10H20O2	000334-48-5	64
3			Nonanoic acid	158	C9H18O2	000112-05-0	53
4			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	52
5			Dodecanoic acid	200	C12H24O2	000143-07-7	50



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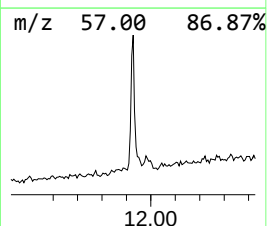
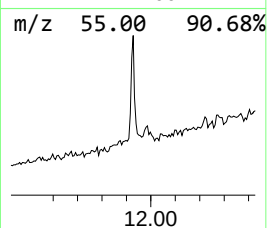
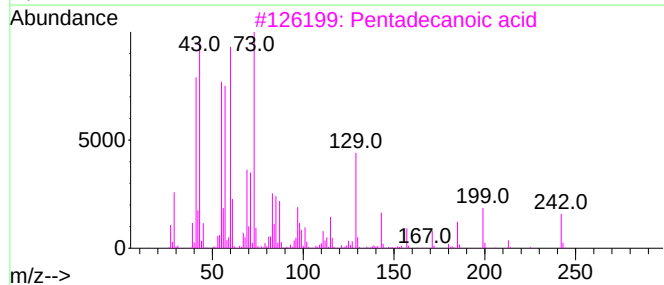
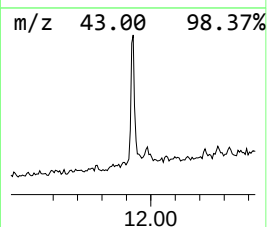
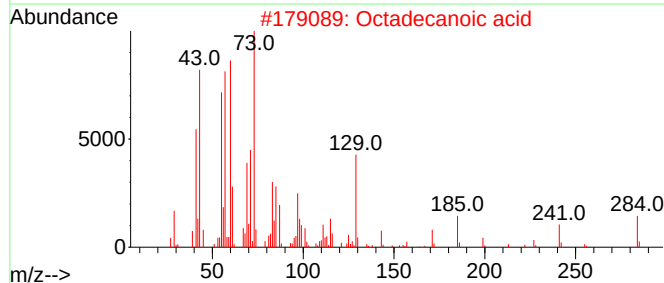
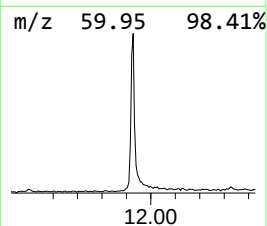
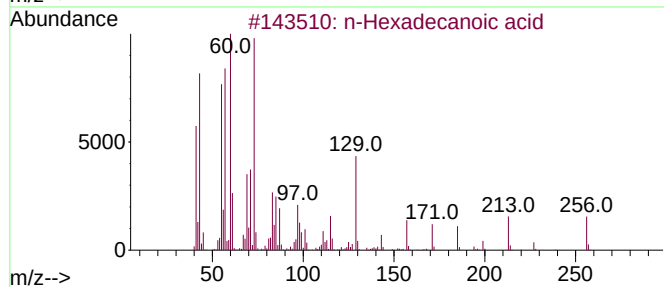
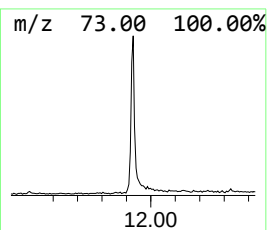
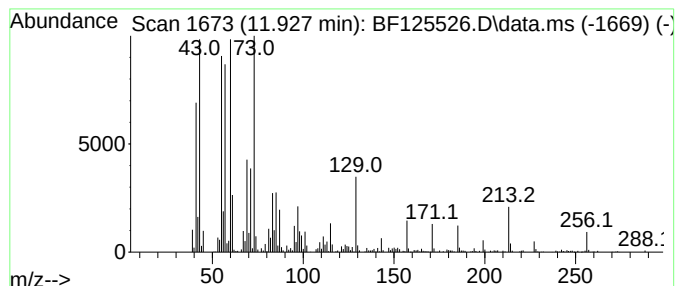
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	13.76 ng	648470	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Undecanoic acid	186	C11H22O2	000112-37-8	81
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125526.D
Acq On : 16 Sep 2021 2:59
Operator : JU/CG
Sample : M3687-27 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A011145

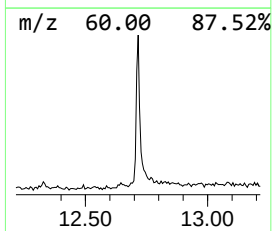
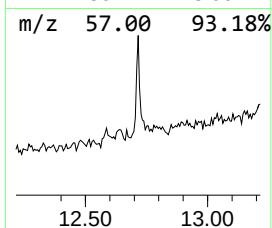
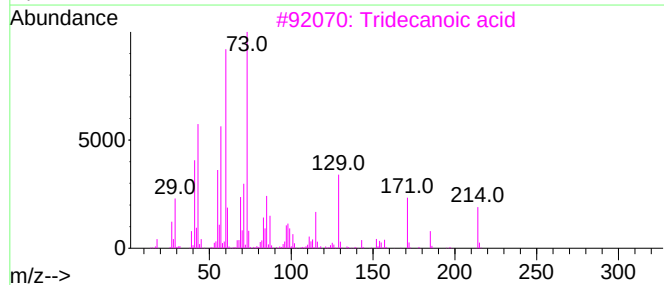
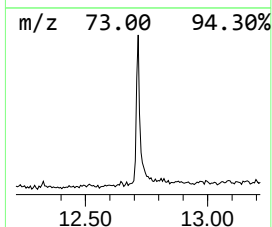
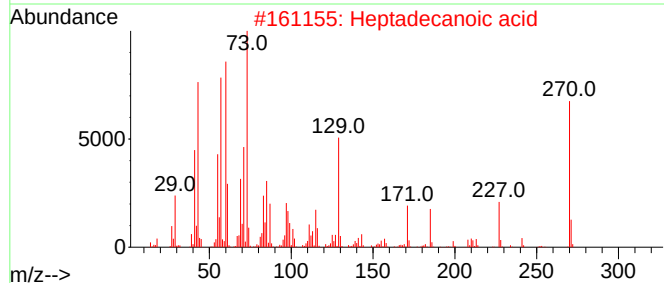
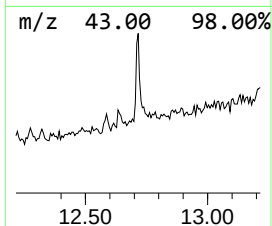
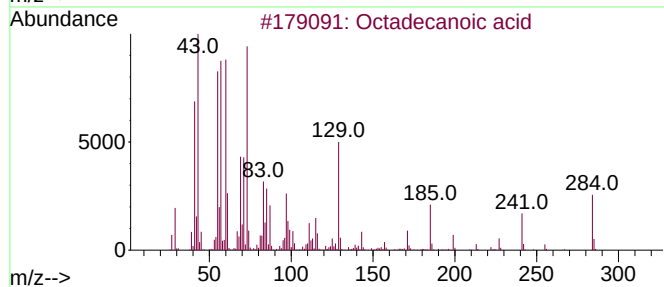
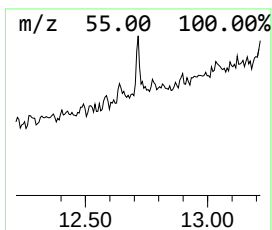
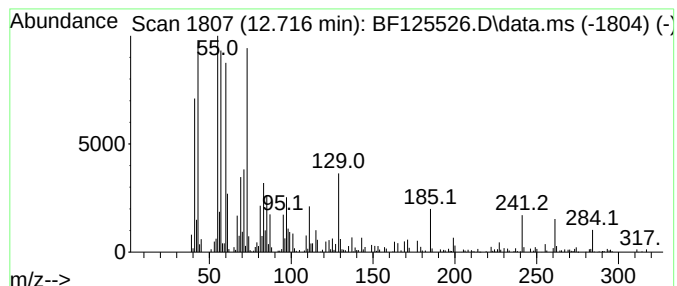
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	7.96 ng	374964	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Heptadecanoic acid	270	C17H34O2	000506-12-7	76
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
Data File : BF125526.D
Acq On : 16 Sep 2021 2:59
Operator : JU/CG
Sample : M3687-27 5X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A011145

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.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
Butane, 2-metho...	2.140	7.0	ng	334551	1	6.869	952150	20.0
2-Pentanone, 4-...	5.069	2.5	ng	117187	1	6.869	952150	20.0
Heptanoic acid	8.510	6.2	ng	356099	2	8.151	1148240	20.0
n-Decanoic acid	9.075	5.8	ng	313683	3	9.910	1079100	20.0
Undecanoic acid	9.604	2.4	ng	130668	3	9.910	1079100	20.0
n-Hexadecanoic ...	11.927	13.8	ng	648470	4	11.398	942473	20.0
Octadecanoic acid	12.716	8.0	ng	374964	4	11.398	942473	20.0