

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
 Data File : BF130990.D
 Acq On : 04 Nov 2022 14:00
 Operator : CG\JU
 Sample : N5335-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-2

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130990.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.287	26	34	40	rVB	1634215	2109698	45.38%	6.956%
2	5.146	516	520	529	rVB	210542	240735	5.18%	0.794%
3	5.534	582	586	589	rBV	1982811	1928882	41.49%	6.360%
4	6.534	751	756	779	rVB	862283	1281586	27.57%	4.226%
5	6.910	816	820	824	rBV	799640	684719	14.73%	2.258%
6	6.969	826	830	833	rBV	146299	156608	3.37%	0.516%
7	7.481	910	917	920	rVB	2109378	2590113	55.72%	8.540%
8	8.098	1018	1022	1034	rBV	145353	338453	7.28%	1.116%
9	8.198	1034	1039	1042	rVB	859507	825404	17.76%	2.722%
10	8.669	1099	1119	1122	rBV	1314565	4648538	100.00%	15.327%
11	9.281	1216	1223	1226	rBV	3828906	4073693	87.63%	13.432%
12	9.957	1332	1338	1342	rVB	1118598	1034359	22.25%	3.411%
13	10.375	1404	1409	1413	rVB	331304	300773	6.47%	0.992%
14	10.757	1466	1474	1477	rBV	2632357	2620483	56.37%	8.640%
15	11.451	1587	1592	1596	rBV	1065032	952166	20.48%	3.140%
16	11.833	1654	1657	1660	rVB	75084	61008	1.31%	0.201%
17	12.404	1748	1754	1766	rBV2	30092	71238	1.53%	0.235%
18	12.692	1801	1803	1807	rVB	80219	63968	1.38%	0.211%
19	12.992	1850	1854	1857	rBV	656961	543984	11.70%	1.794%
20	13.051	1858	1864	1867	rVV	3926148	3854106	82.91%	12.708%
21	13.422	1922	1927	1935	rBV2	38780	85374	1.84%	0.281%
22	13.821	1991	1995	1998	rBV	99288	92261	1.98%	0.304%
23	14.004	2022	2026	2039	rBV5	78697	242690	5.22%	0.800%
24	14.104	2039	2043	2047	rVB	898141	777513	16.73%	2.564%
25	14.198	2053	2059	2063	rBV	84710	112619	2.42%	0.371%
26	14.333	2076	2082	2089	rBV2	27966	70662	1.52%	0.233%
27	15.610	2294	2299	2306	rVB	444960	566767	12.19%	1.869%

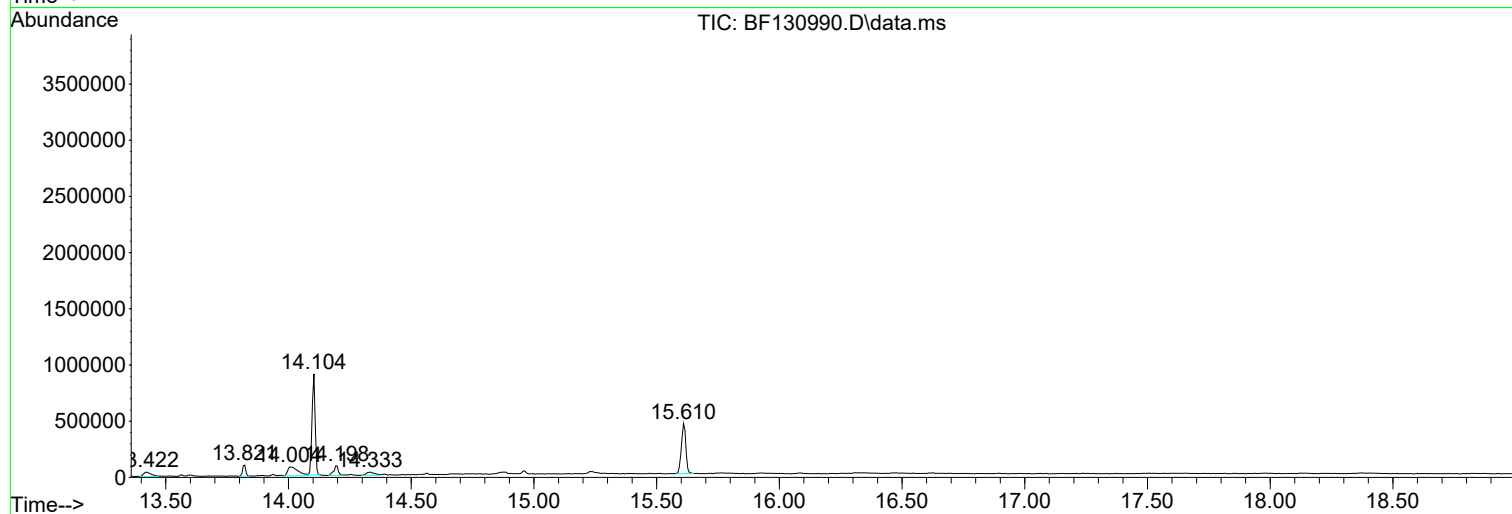
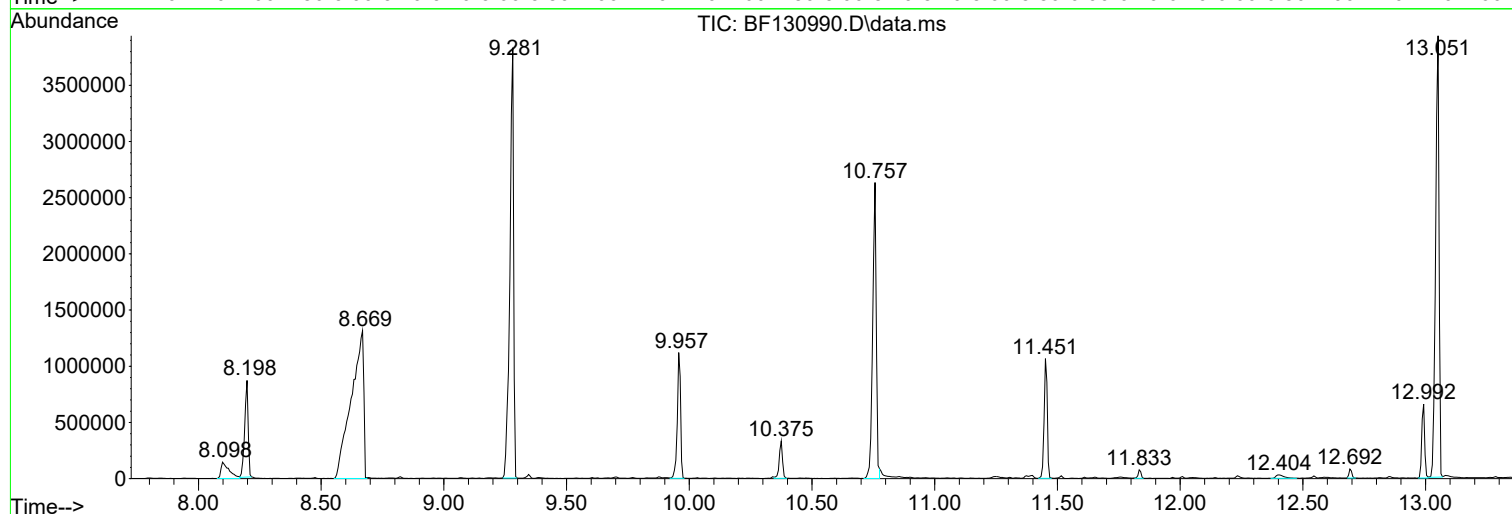
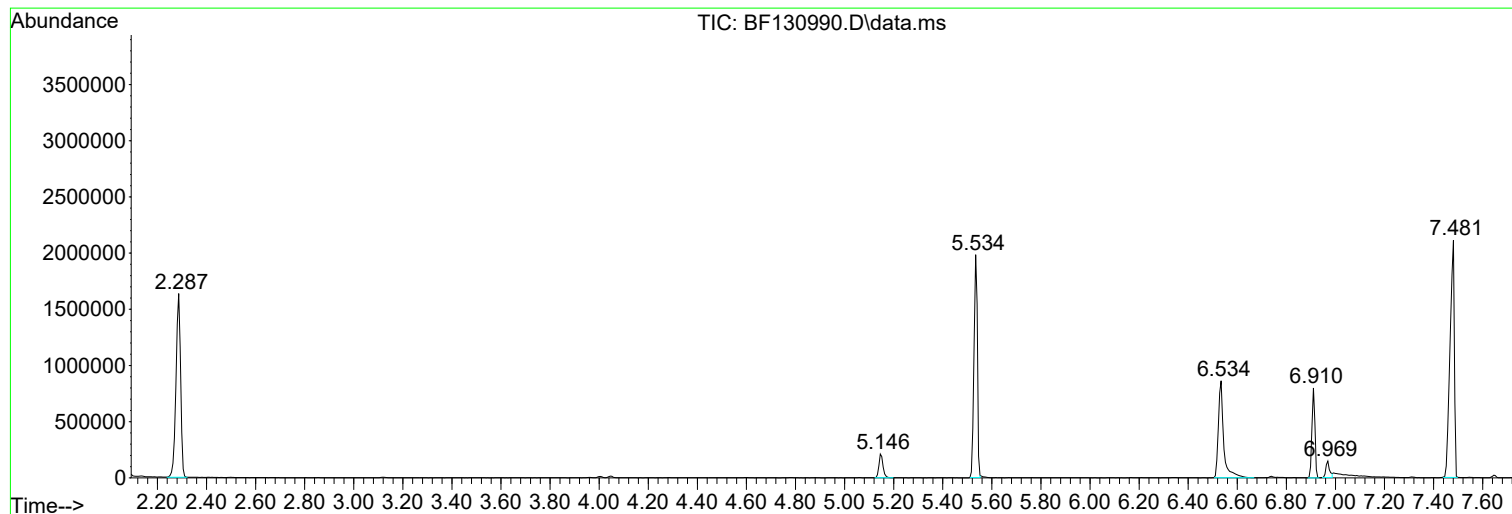
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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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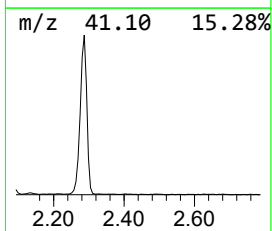
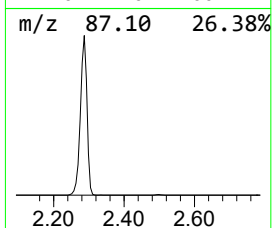
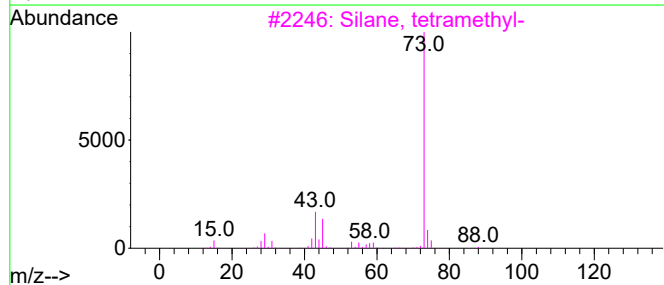
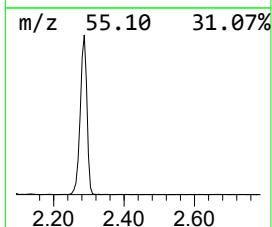
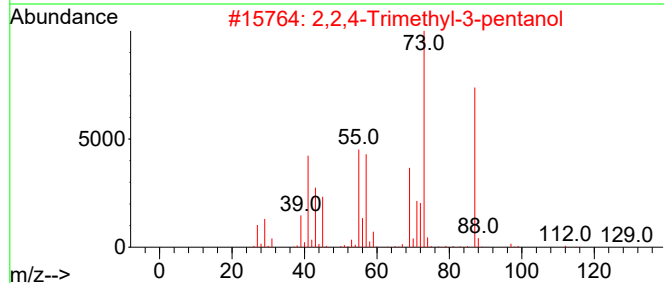
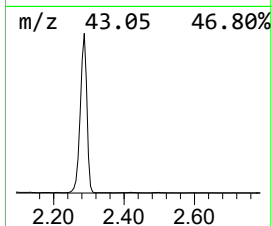
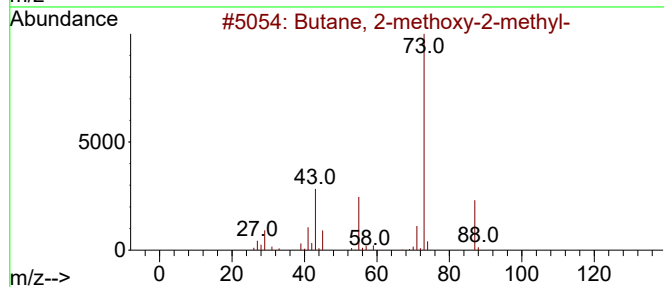
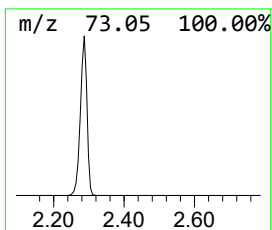
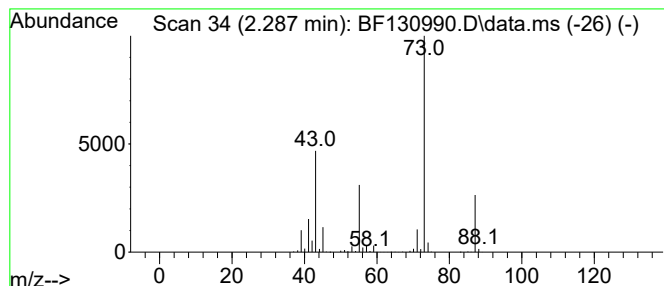
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	61.62 ng	2109700	1,4-Dichlorobenzene-d4	6.910

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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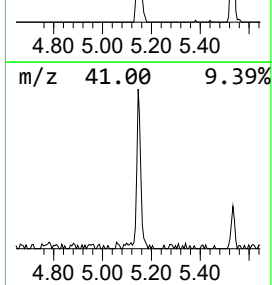
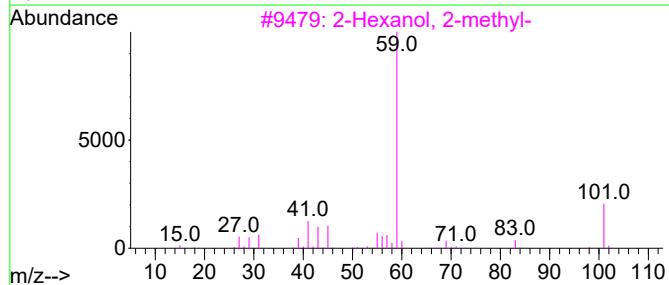
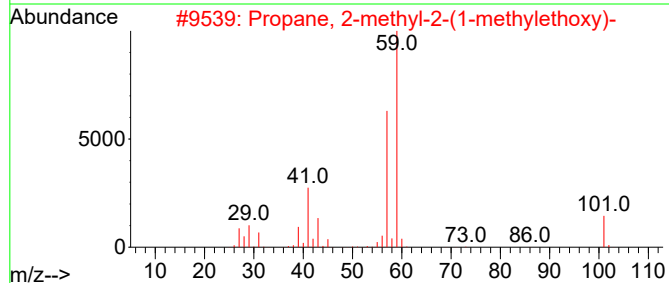
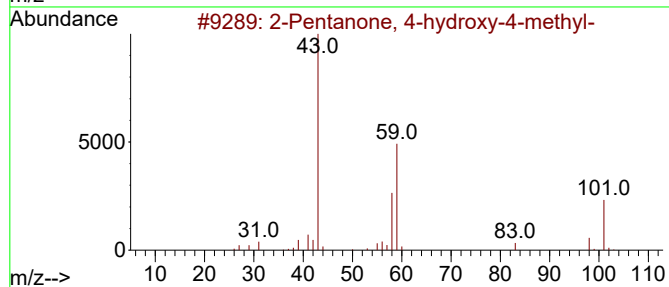
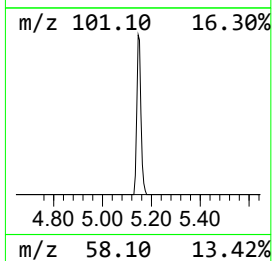
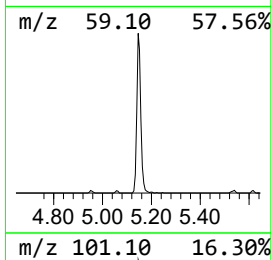
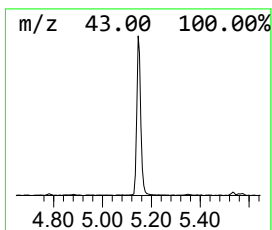
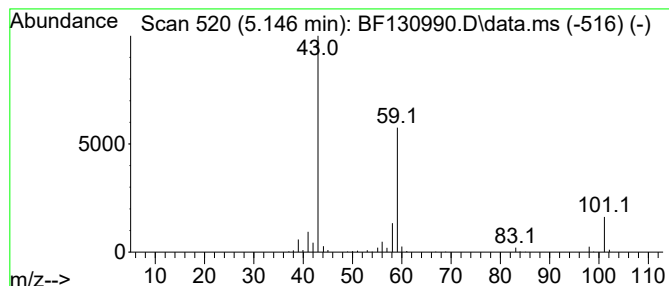
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.146	7.03 ng	240735	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		



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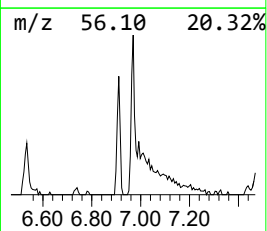
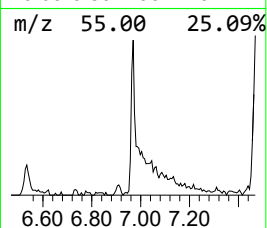
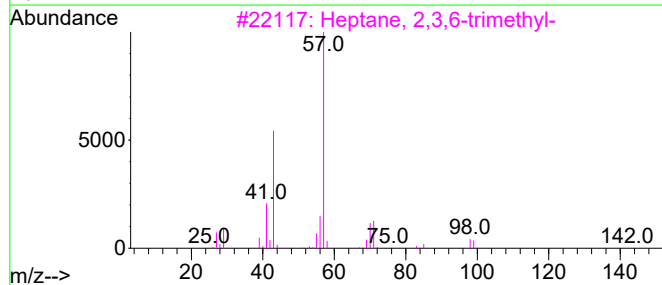
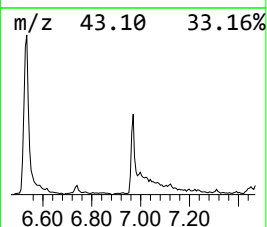
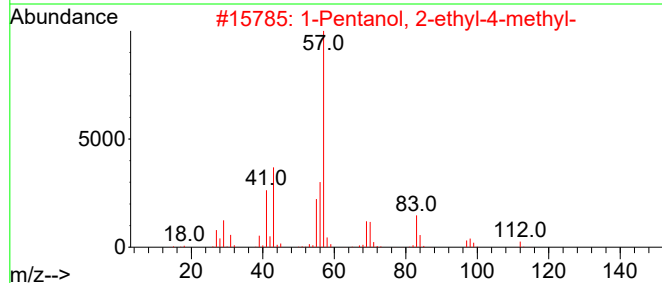
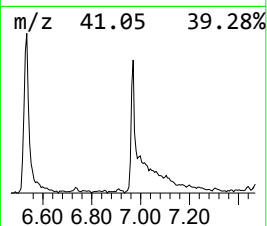
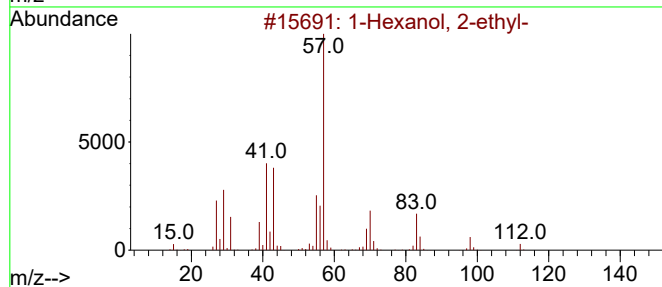
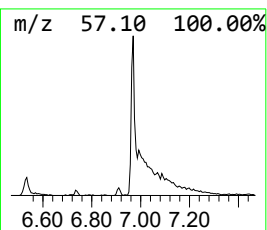
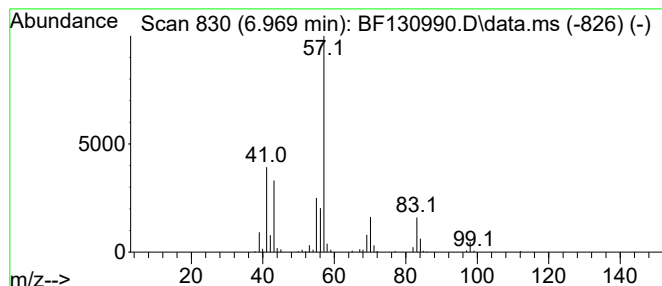
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.969	4.57 ng	156608	1,4-Dichlorobenzene-d4	6.910

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	83
3			Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	64
4			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	59
5			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56



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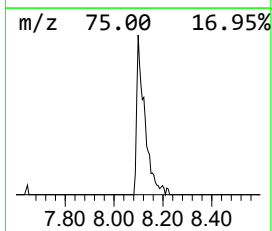
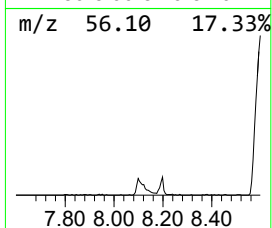
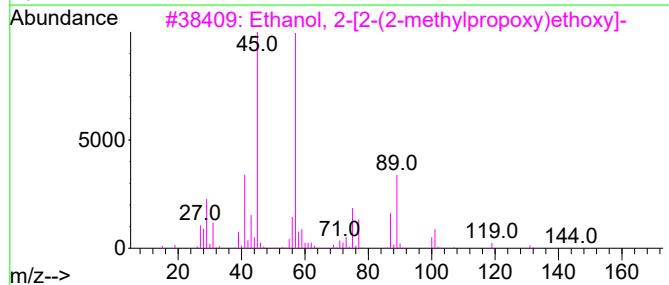
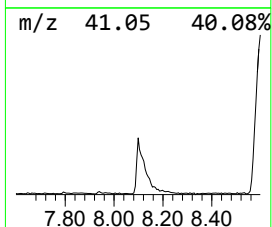
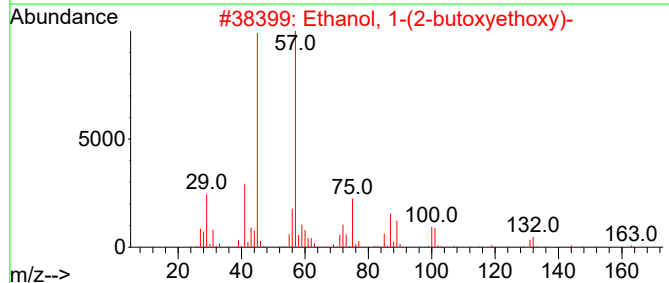
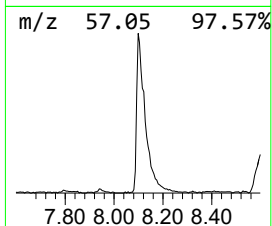
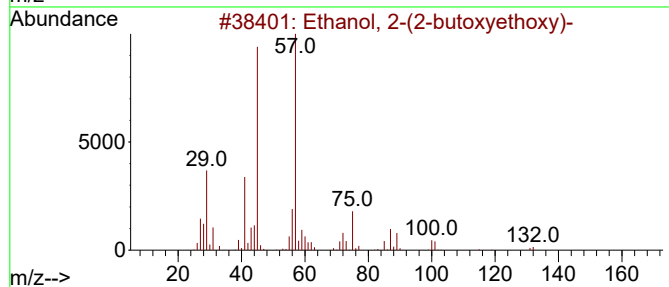
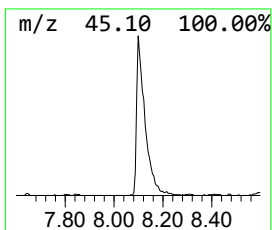
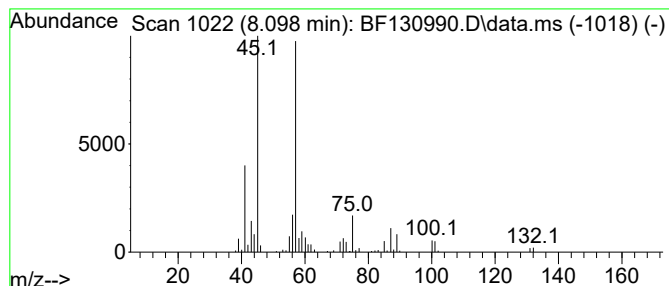
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	8.20 ng	338453	Naphthalene-d8	8.198

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	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	53



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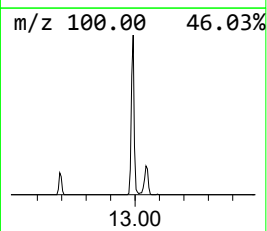
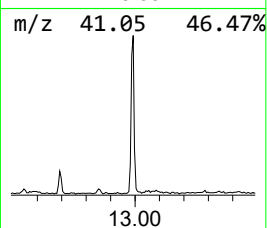
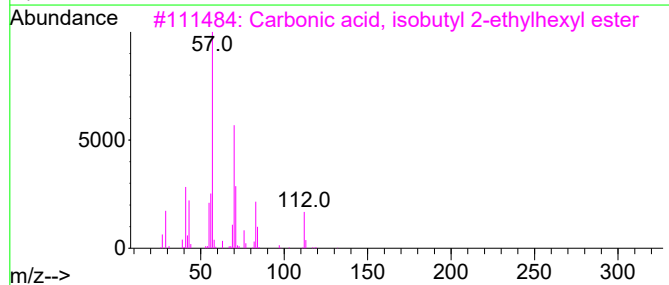
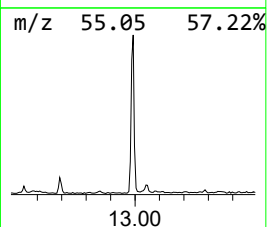
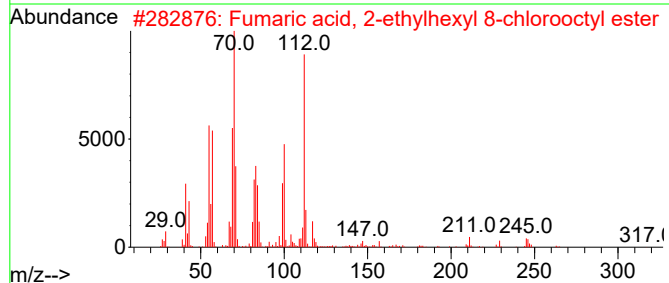
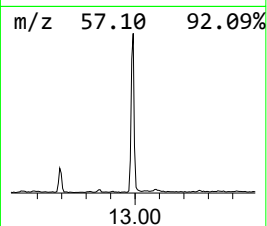
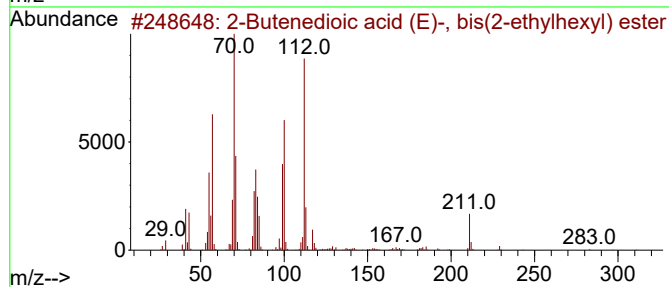
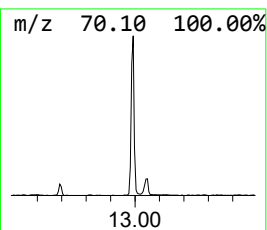
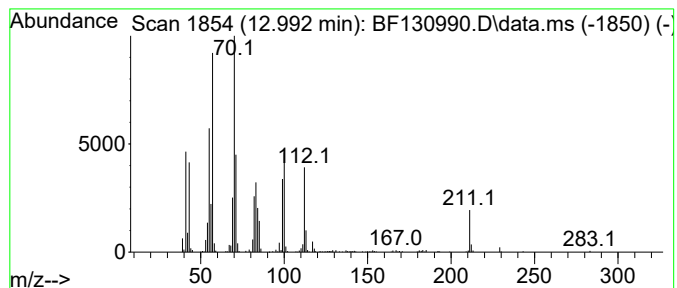
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Peak Number 5 2-Butenedioic acid (E)-, bi... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.992	13.99 ng	543984	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butenedioic acid (E)-, bis(2-e...	340	C20H36O4	000141-02-6	91
2			Fumaric acid, 2-ethylhexyl 8-chl...	374	C20H35ClO4	1000405-57-8	59
3			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	50
4			Carbonic acid, bis(2-ethylhexyl)...	286	C17H34O3	014858-73-2	27
5			Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	27



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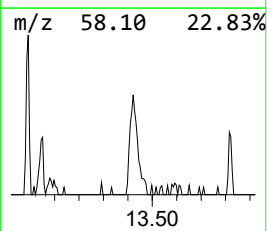
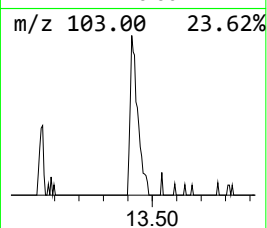
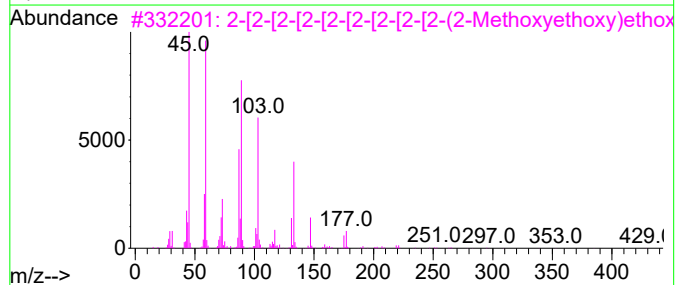
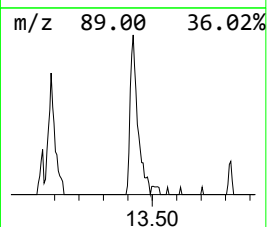
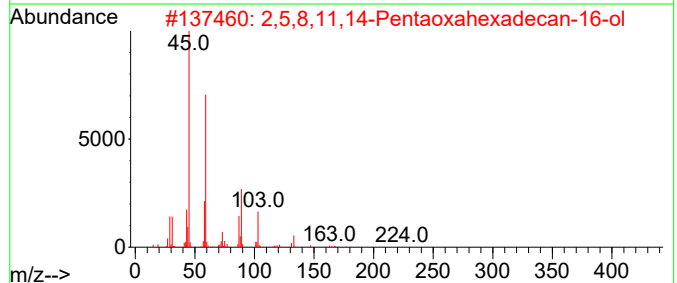
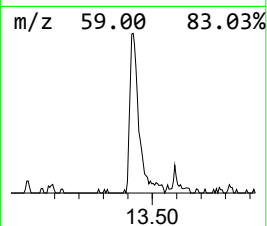
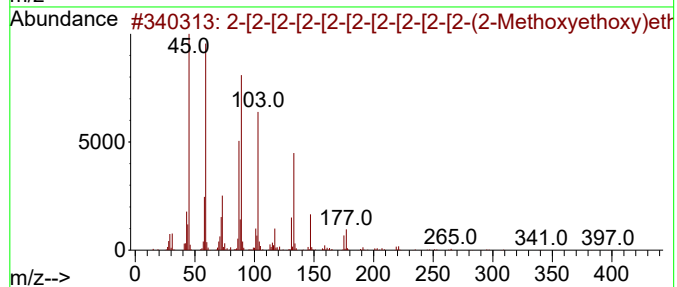
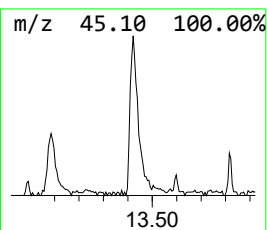
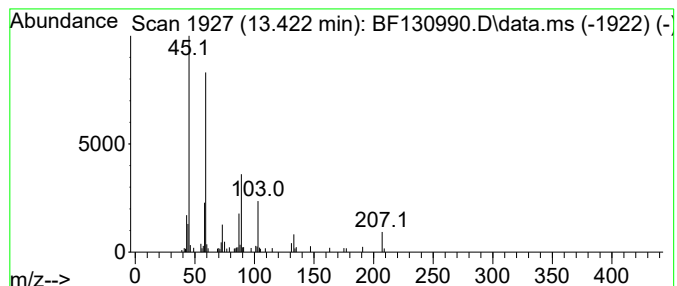
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-[2-[2-[2-[2-[2-[2-[2-[... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.422	2.20 ng	85374	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-(2-...	516	C23H48O12	1010352-04-4	91		
2	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	91		
3	2-[2-[2-[2-[2-[2-[2-[2-(2-Met...	472	C21H44O11	027425-92-9	91		
4	2-[2-[2-[2-[2-[2-(2-Methoxyethox...	340	C15H32O8	004437-01-8	90		
5	2-[2-[2-[2-[2-[2-[2-(2-Methox...	428	C19H40O10	006048-68-6	90		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF130990.D
Acq On : 04 Nov 2022 14:00
Operator : CG\JU
Sample : N5335-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2

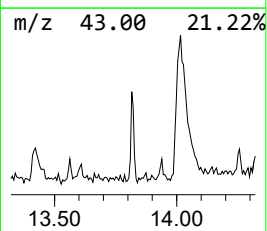
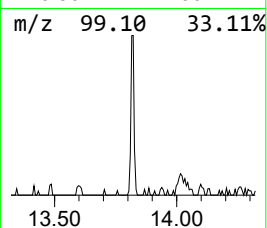
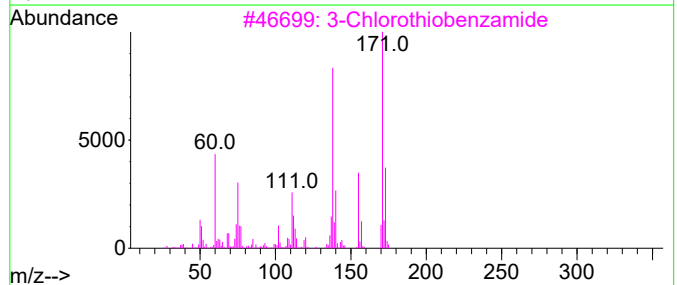
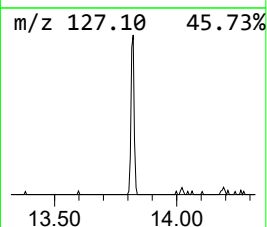
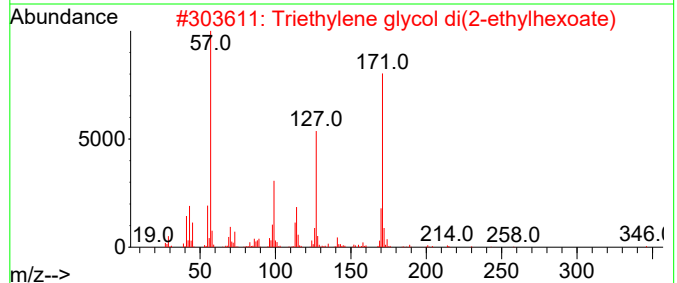
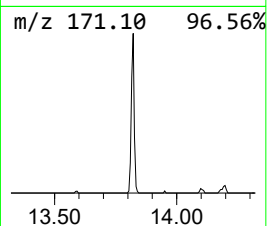
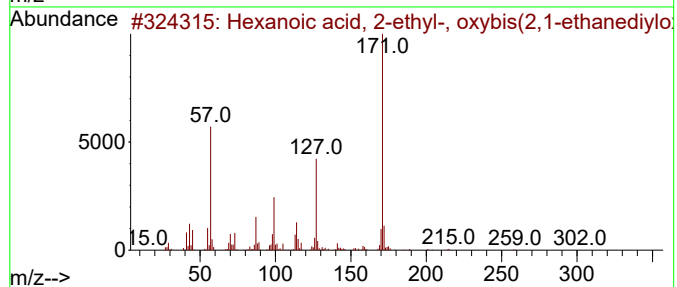
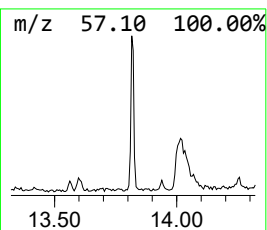
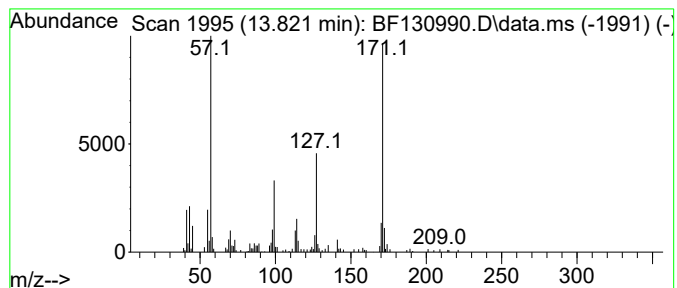
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexanoic acid, 2-ethyl-, ox... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.822	2.37 ng	92261	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-, oxybis(...	446	C24H46O7	018268-70-7	91
2			Triethylene glycol di(2-ethylhex...	402	C22H42O6	000094-28-0	81
3			3-Chlorothiobenzamide	171	C7H6ClNS	002548-79-0	43
4			Adipic acid, 4-heptyl propyl ester	286	C16H30O4	1000349-73-5	35
5			3,4-Dichlorobenzonitrile	171	C7H3Cl2N	006574-99-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF130990.D
Acq On : 04 Nov 2022 14:00
Operator : CG\JU
Sample : N5335-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2

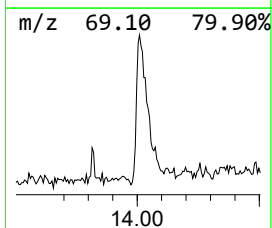
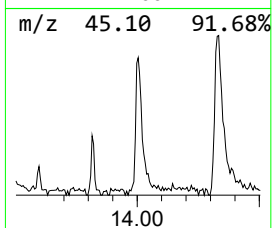
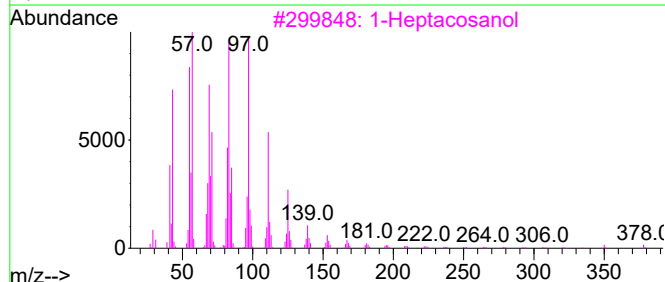
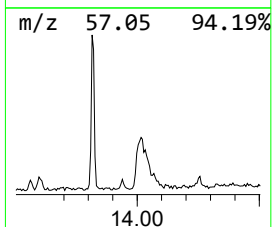
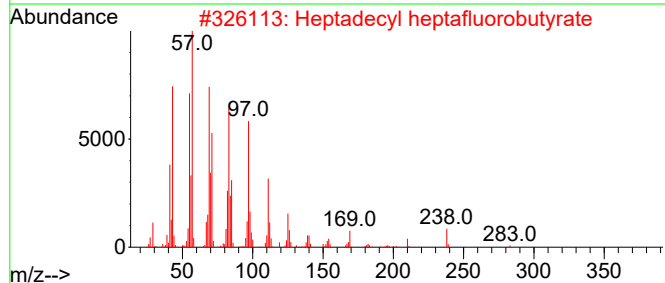
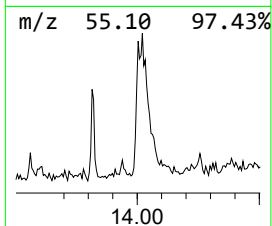
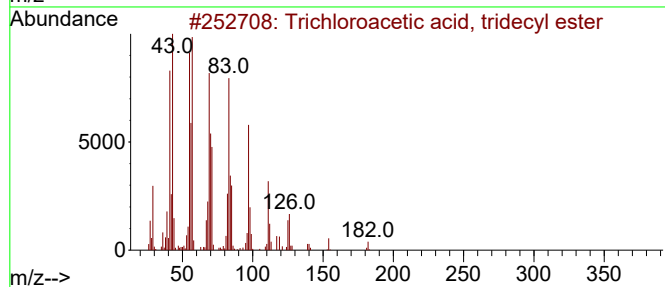
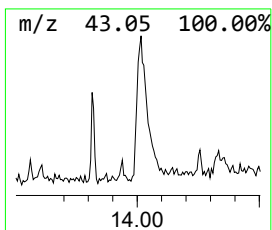
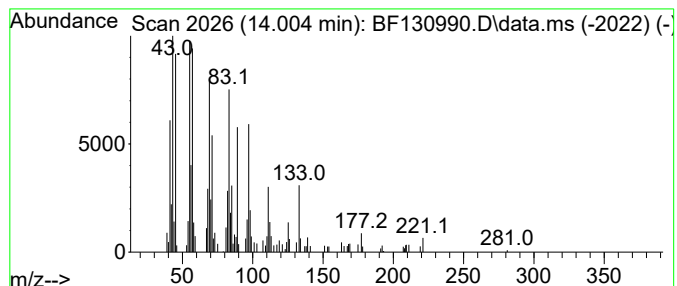
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, tride... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	6.24 ng	242690	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	64
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
3			1-Heptacosanol	396	C27H56O	002004-39-9	64
4			Dichloroacetic acid, tridecyl ester	310	C15H28Cl2O2	1000280-48-3	58
5			2-Pentadecanol	228	C15H32O	001653-34-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF130990.D
Acq On : 04 Nov 2022 14:00
Operator : CG\JU
Sample : N5335-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2

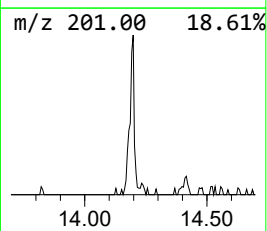
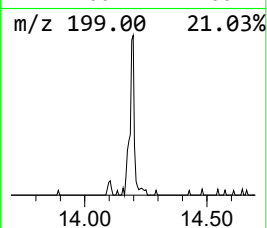
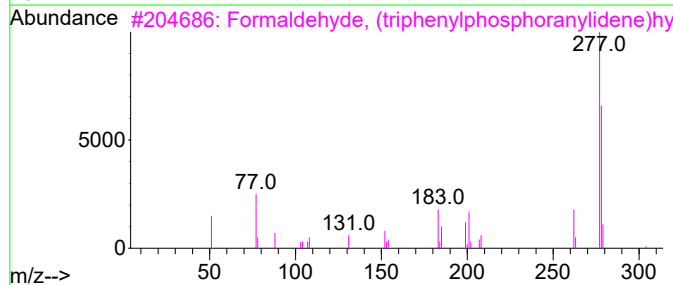
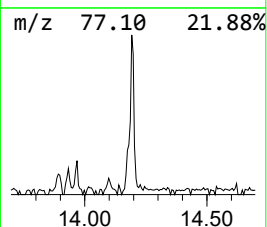
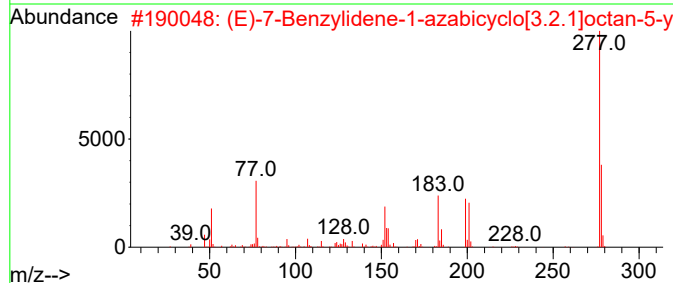
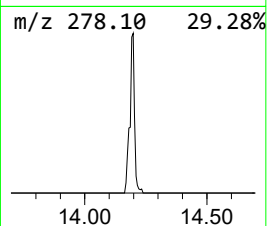
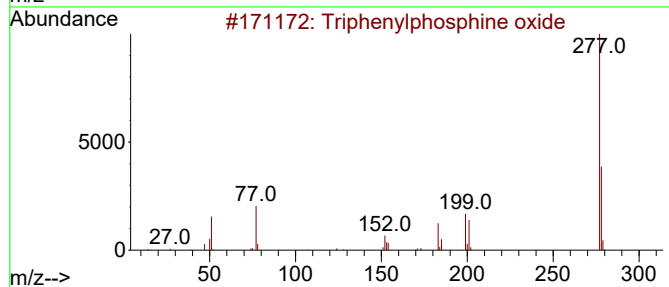
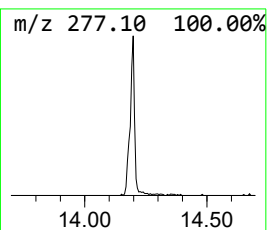
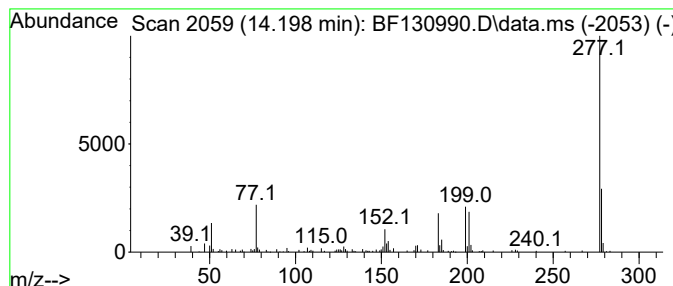
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triphenylphosphine oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	2.90 ng	112619	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	47
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	45
4			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	43
5			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110422\
Data File : BF130990.D
Acq On : 04 Nov 2022 14:00
Operator : CG\JU
Sample : N5335-06
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.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...	2.287	61.6	ng	2109700	1	6.910	684719	20.0
2-Pentanone, 4-...	5.146	7.0	ng	240735	1	6.910	684719	20.0
1-Hexanol, 2-et...	6.969	4.6	ng	156608	1	6.910	684719	20.0
Ethanol, 2-(2-b...	8.098	8.2	ng	338453	2	8.198	825404	20.0
2-Butenedioic a...	12.992	14.0	ng	543984	5	14.104	777513	20.0
2-[2-[2-[2-[2-...	13.422	2.2	ng	85374	5	14.104	777513	20.0
Hexanoic acid, ...	13.822	2.4	ng	92261	5	14.104	777513	20.0
Trichloroacetic...	14.004	6.2	ng	242690	5	14.104	777513	20.0
Triphenylphosph...	14.198	2.9	ng	112619	5	14.104	777513	20.0