

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
 Data File : BF131123.D
 Acq On : 10 Nov 2022 14:59
 Operator : CG\JU
 Sample : N5494-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-19

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-BF110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131123.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	8	15	22	rVB	654910	824331	41.07%	5.577%
2	2.287	29	34	38	rBV	34251	43696	2.18%	0.296%
3	4.493	405	409	417	rVB	80725	91823	4.57%	0.621%
4	5.116	509	515	526	rVB	557567	719703	35.86%	4.869%
5	5.510	577	582	585	rBV	2087137	1869067	93.12%	12.645%
6	5.904	646	649	652	rBV	32634	27095	1.35%	0.183%
7	6.516	748	753	756	rBV	1893540	1816016	90.47%	12.286%
8	6.887	812	816	819	rBV	577581	445980	22.22%	3.017%
9	7.451	907	912	915	rBV	1231799	1162575	57.92%	7.865%
10	8.169	1030	1034	1038	rBV	601596	568543	28.32%	3.846%
11	9.251	1213	1218	1221	rBV	2162704	2007259	100.00%	13.580%
12	9.933	1329	1334	1337	rBV	730050	635905	31.68%	4.302%
13	10.727	1464	1469	1472	rBV	1210273	1179721	58.77%	7.981%
14	11.427	1584	1588	1591	rBV	726425	619058	30.84%	4.188%
15	12.639	1790	1794	1798	rVB	26529	24792	1.24%	0.168%
16	12.874	1827	1834	1837	rBV	22681	28504	1.42%	0.193%
17	13.016	1854	1858	1861	rBV	1835321	1550497	77.24%	10.490%
18	13.974	2014	2021	2030	rBV6	34503	105979	5.28%	0.717%
19	14.074	2034	2038	2041	rVV	494788	425907	21.22%	2.881%
20	14.168	2048	2054	2059	rBV	74741	81764	4.07%	0.553%
21	14.921	2178	2182	2189	rBV	60332	66137	3.29%	0.447%
22	15.127	2214	2217	2220	rBV	18991	23204	1.16%	0.157%
23	15.574	2287	2293	2299	rBV	350184	463685	23.10%	3.137%

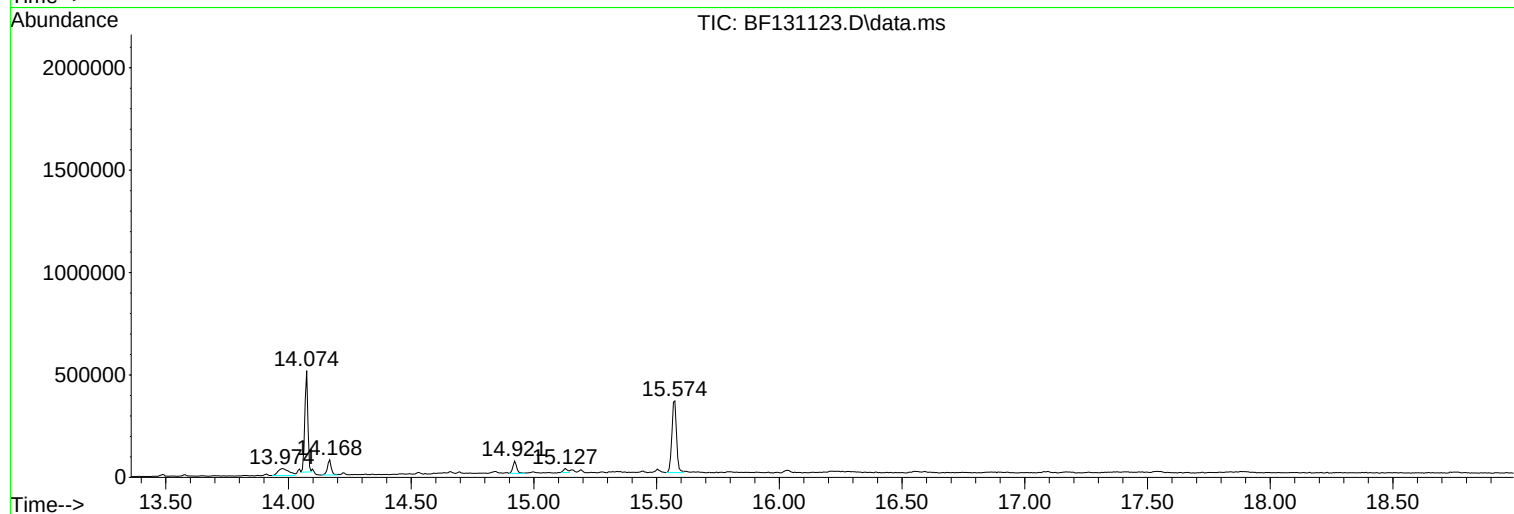
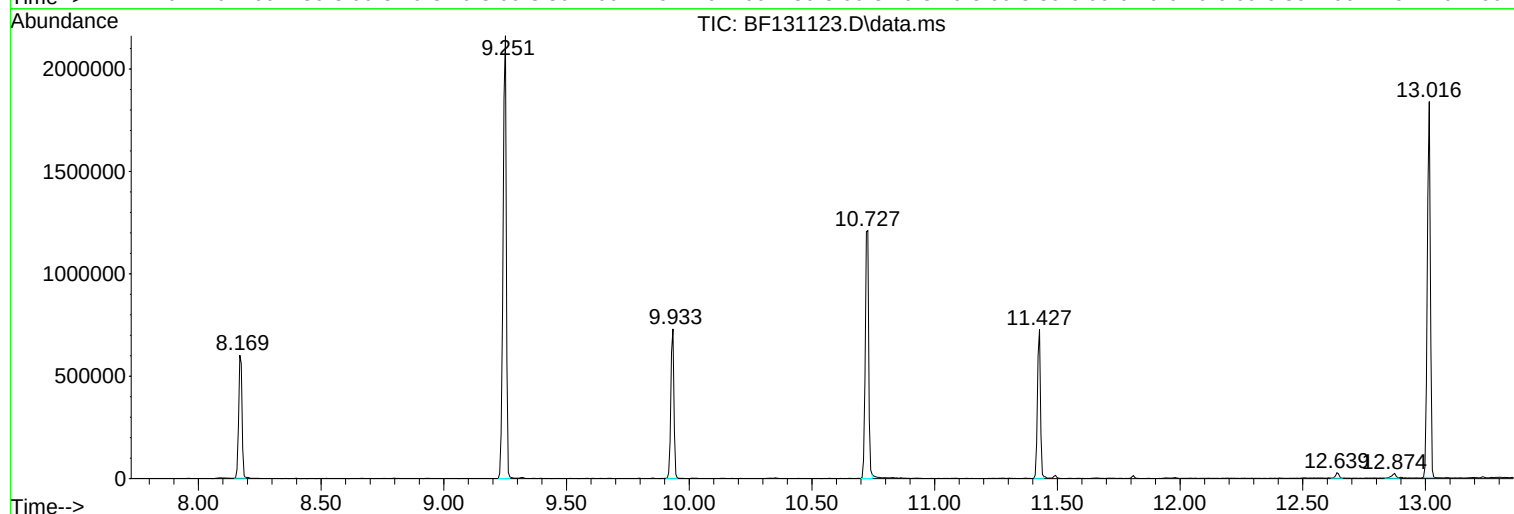
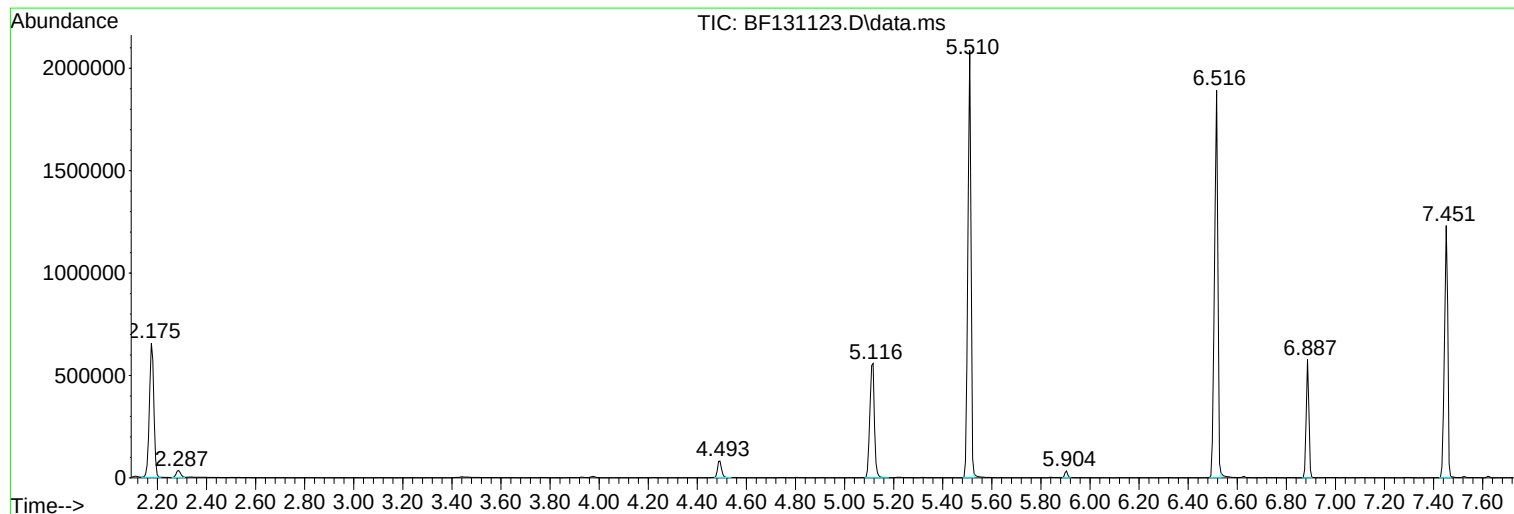
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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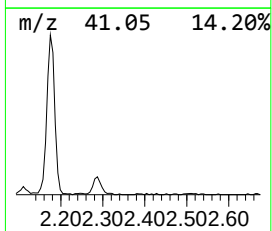
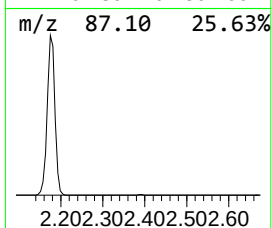
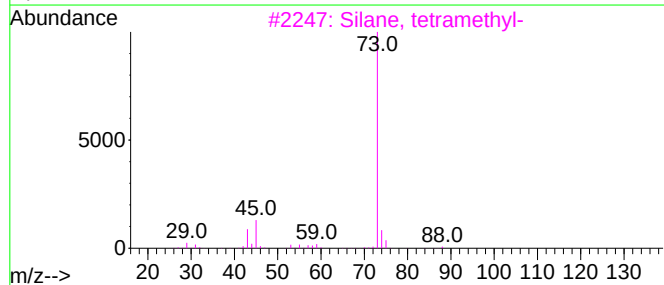
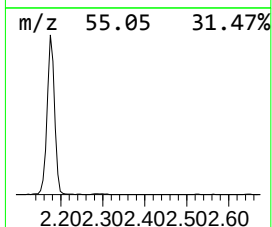
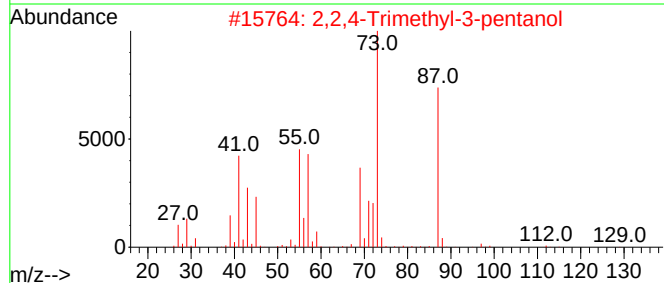
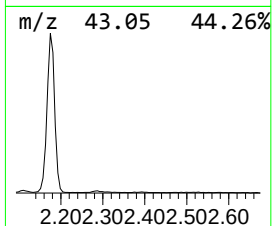
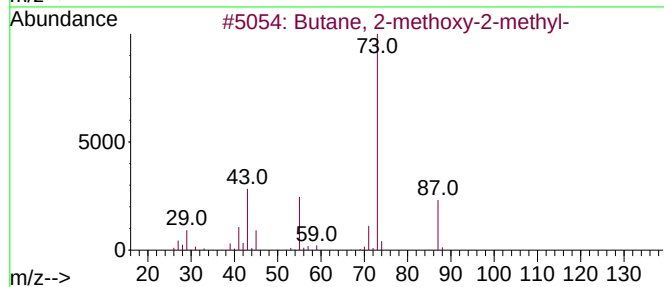
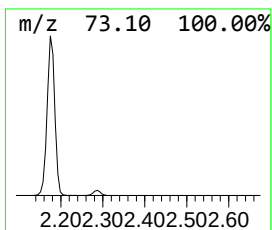
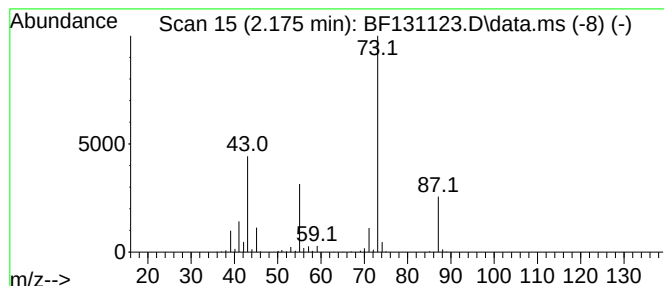
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	36.97 ng	824331	1,4-Dichlorobenzene-d4	6.886

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	38
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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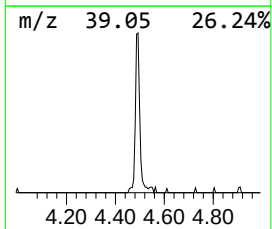
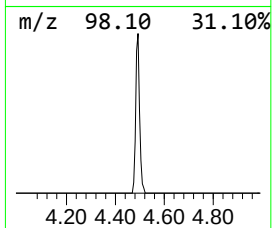
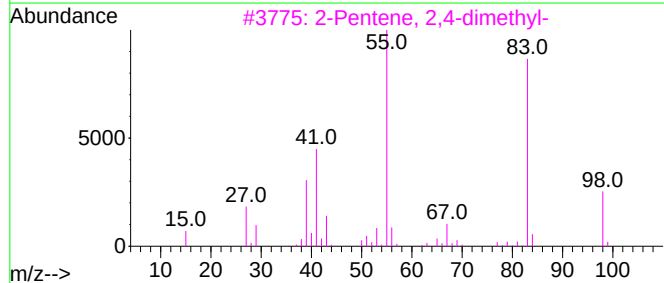
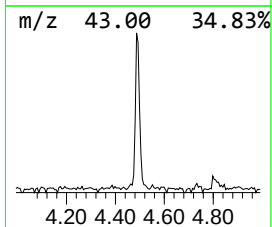
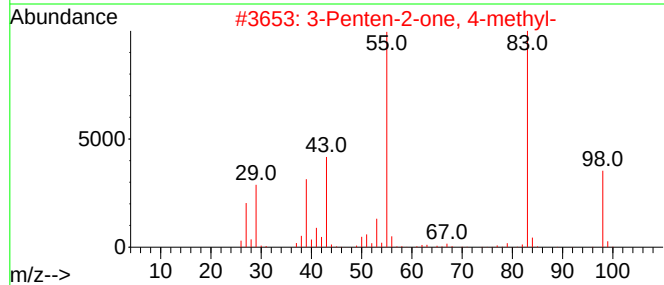
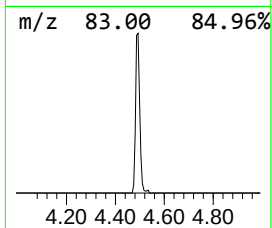
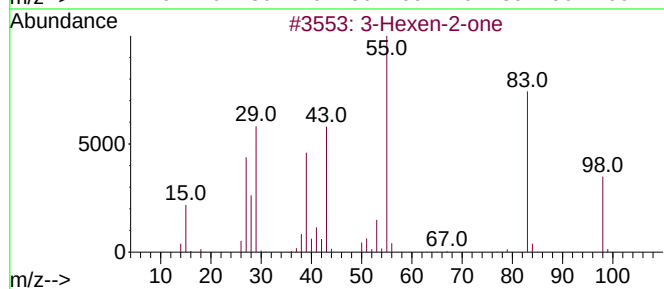
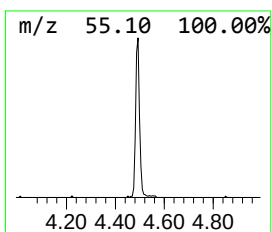
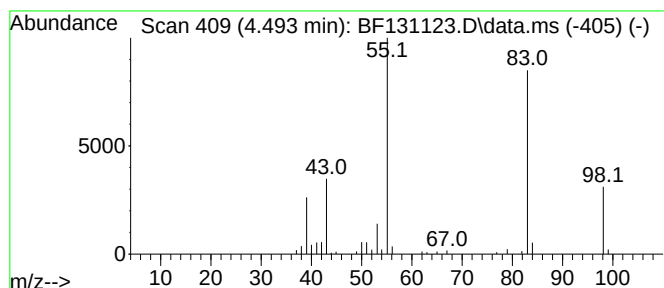
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.493	4.12 ng	91823	1,4-Dichlorobenzene-d4	6.886

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Hexen-2-one	98	C6H10O	000763-93-9	91
2		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86



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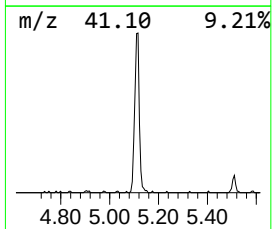
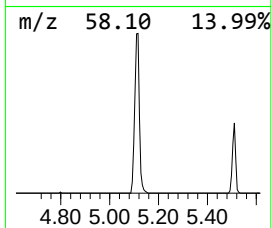
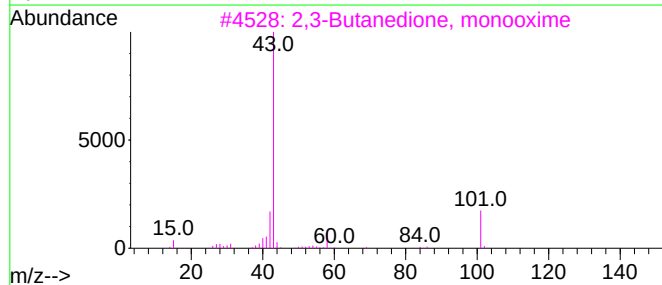
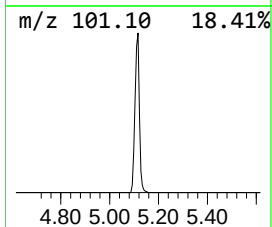
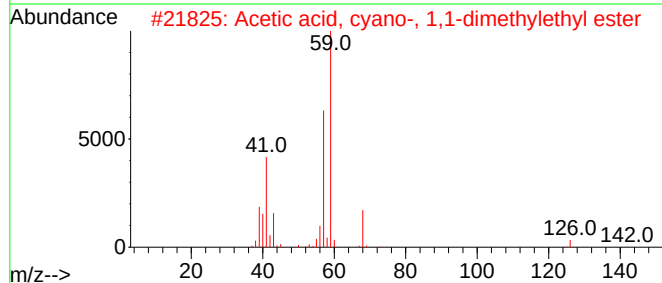
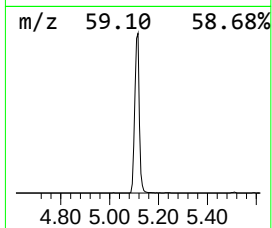
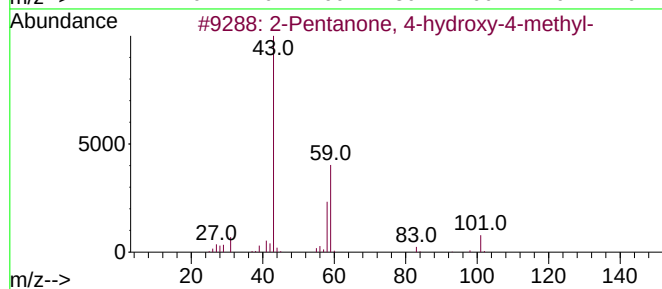
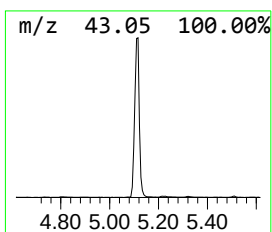
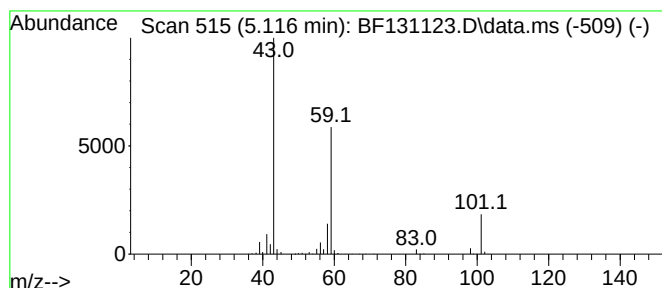
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	32.28 ng	719703	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9



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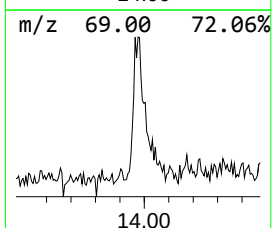
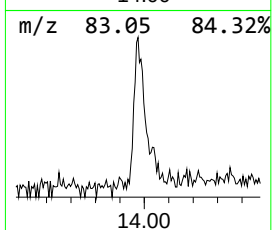
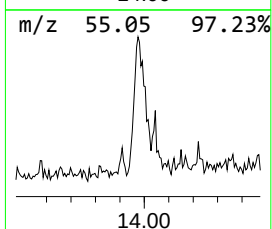
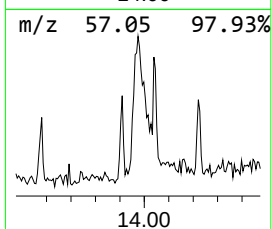
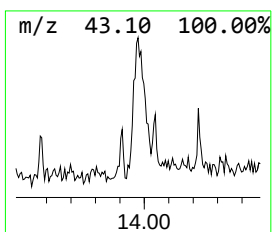
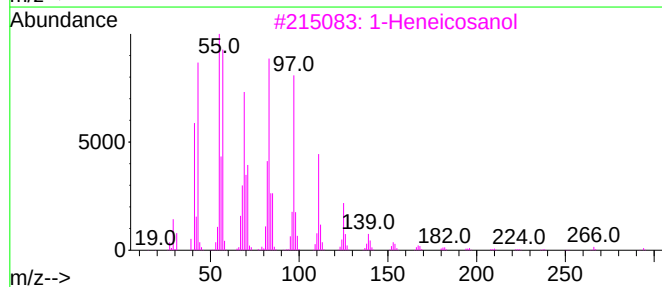
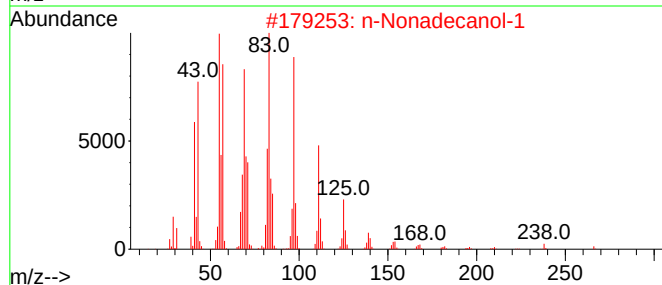
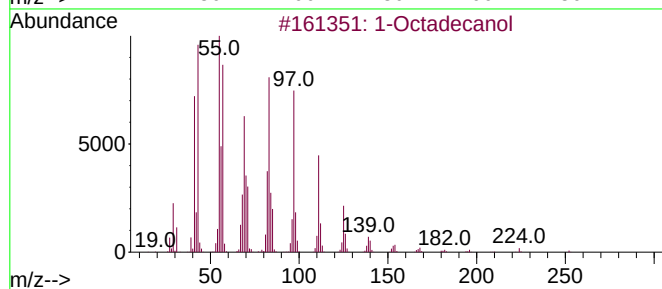
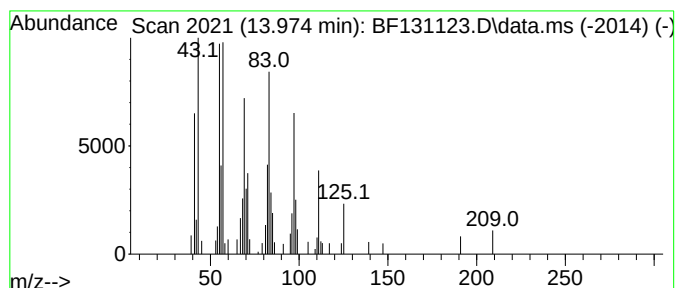
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Octadecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	4.98 ng	105979	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanol	270	C18H38O	000112-92-5	90
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	90
3			1-Heneicosanol	312	C21H44O	015594-90-8	86
4			Behenic alcohol	326	C22H46O	000661-19-8	86
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	83



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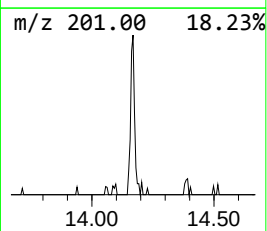
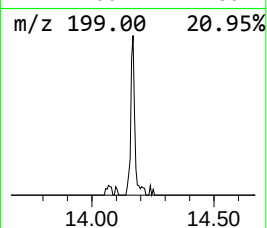
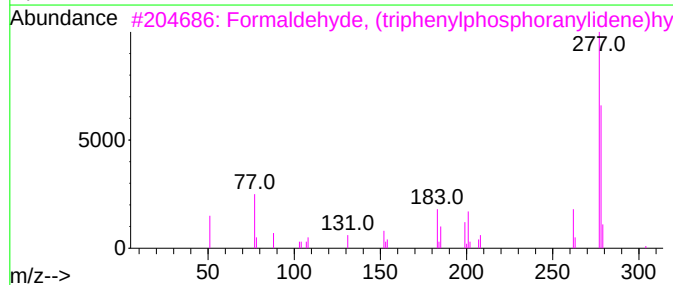
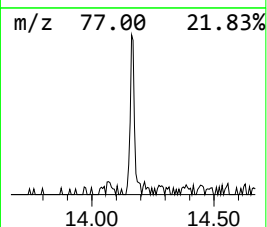
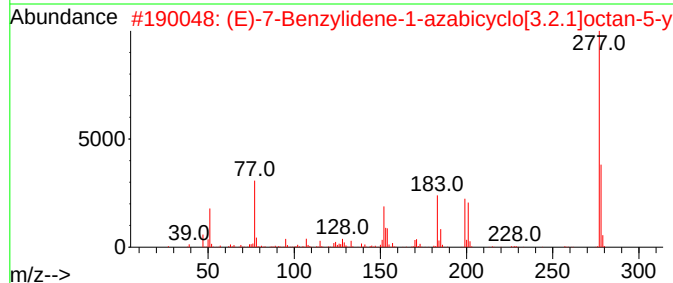
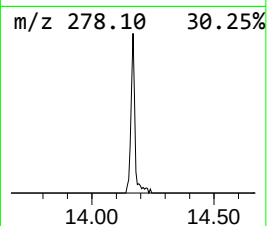
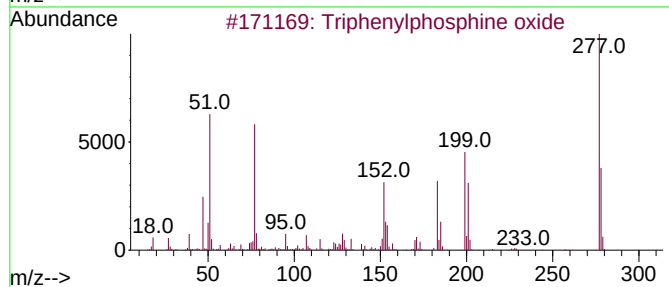
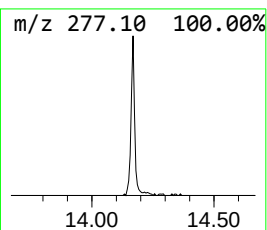
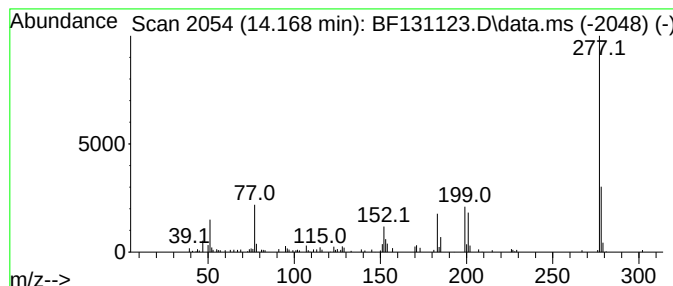
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.168	3.84 ng	81764	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	62
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	43
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	40



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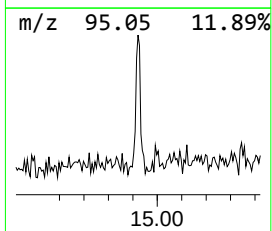
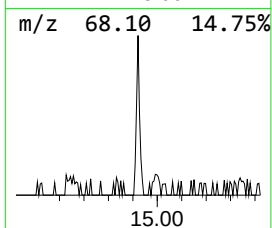
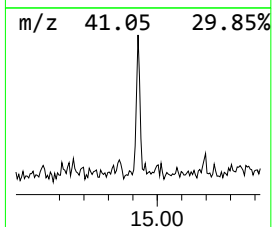
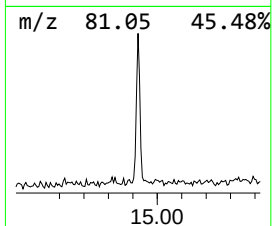
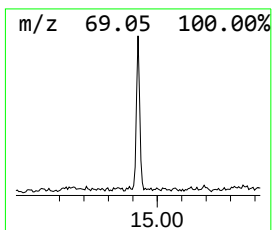
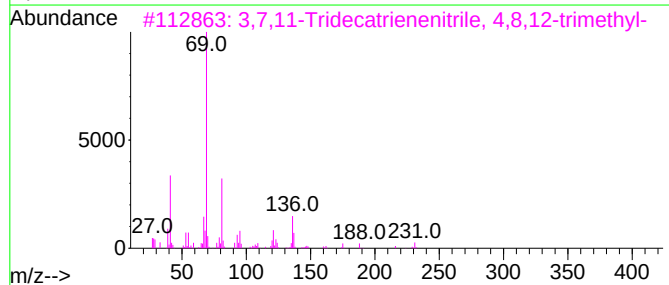
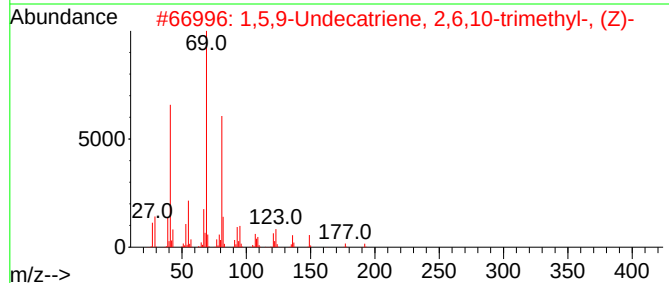
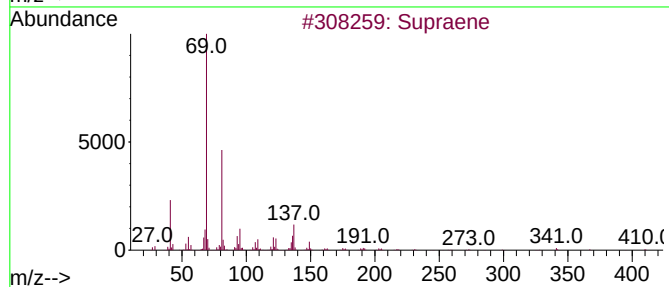
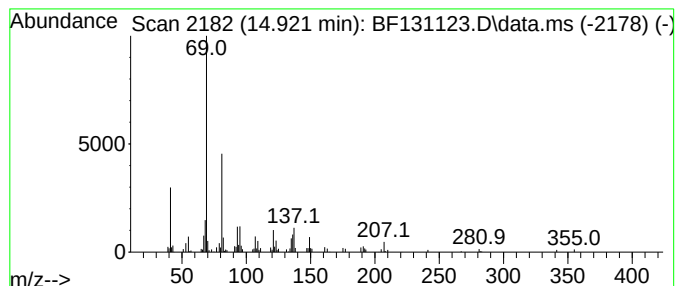
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	2.85 ng	66137	Perylene-d12	15.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
3			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	72
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5			(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131123.D
Acq On : 10 Nov 2022 14:59
Operator : CG\JU
Sample : N5494-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-19

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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...	2.175	37.0	ng	824331	1	6.886	445980	20.0
3-Hexen-2-one	4.493	4.1	ng	91823	1	6.886	445980	20.0
2-Pentanone, 4-...	5.116	32.3	ng	719703	1	6.886	445980	20.0
1-Octadecanol	13.974	5.0	ng	105979	5	14.074	425907	20.0
Triphenylphosph...	14.168	3.8	ng	81764	5	14.074	425907	20.0
Supraene	14.921	2.9	ng	66137	6	15.574	463685	20.0