

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
 Data File : BF131102.D
 Acq On : 09 Nov 2022 23:06
 Operator : CG\JU
 Sample : N5441-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 5486-6

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: BF131102.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	9	15	20	rVB	1715044	2112416	76.50%	12.814%
2	4.493	406	409	414	rVB	73701	78950	2.86%	0.479%
3	5.104	510	513	521	rVB	202959	202693	7.34%	1.230%
4	5.504	577	581	591	rBV	987536	889571	32.22%	5.396%
5	6.510	749	752	764	rBV	712330	627465	22.72%	3.806%
6	6.893	813	817	820	rBV	641982	568222	20.58%	3.447%
7	7.457	907	913	916	rBV	1807618	1772385	64.19%	10.751%
8	8.175	1030	1035	1038	rBV	889223	743409	26.92%	4.510%
9	9.251	1213	1218	1221	rBV	3192022	2761272	100.00%	16.750%
10	9.934	1329	1334	1337	rBV	1019620	814256	29.49%	4.939%
11	10.722	1464	1468	1472	rBV	1474942	1422707	51.52%	8.630%
12	11.422	1584	1587	1591	rBV	917623	838490	30.37%	5.086%
13	13.016	1853	1858	1861	rBV	2476646	2237256	81.02%	13.571%
14	13.922	2007	2012	2023	rBV2	88615	164215	5.95%	0.996%
15	14.069	2034	2037	2041	rBV	720661	613089	22.20%	3.719%
16	14.163	2048	2053	2058	rBV	86874	91149	3.30%	0.553%
17	14.916	2179	2181	2185	rVB2	38595	38136	1.38%	0.231%
18	15.563	2286	2291	2302	rVB	419907	509592	18.45%	3.091%

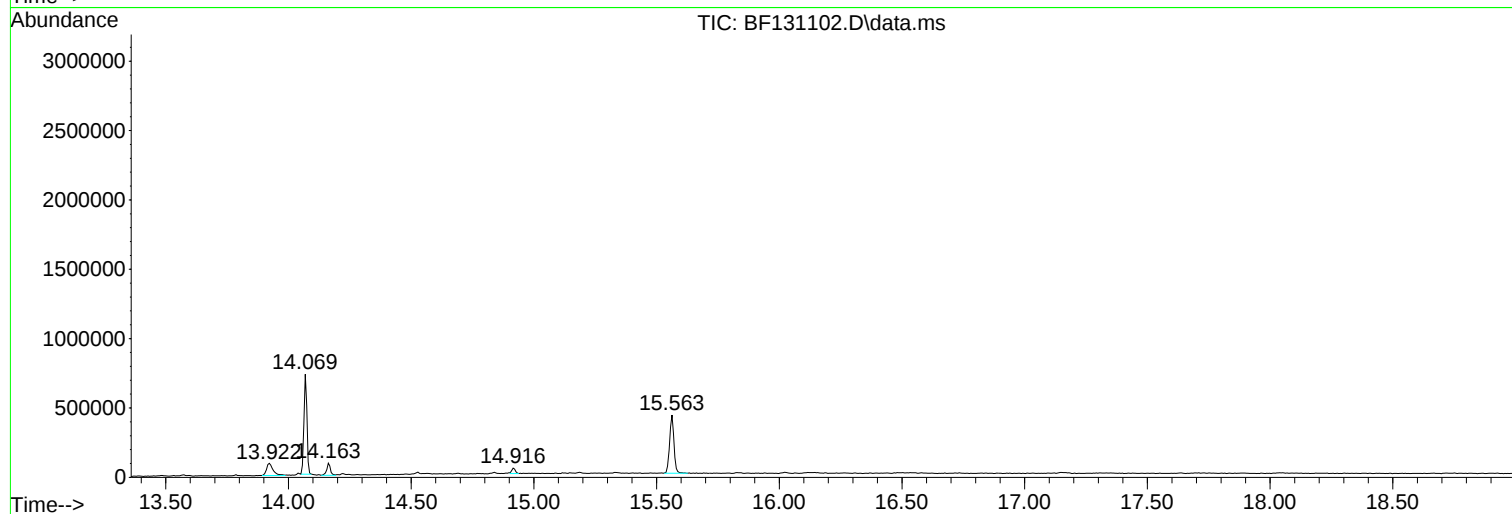
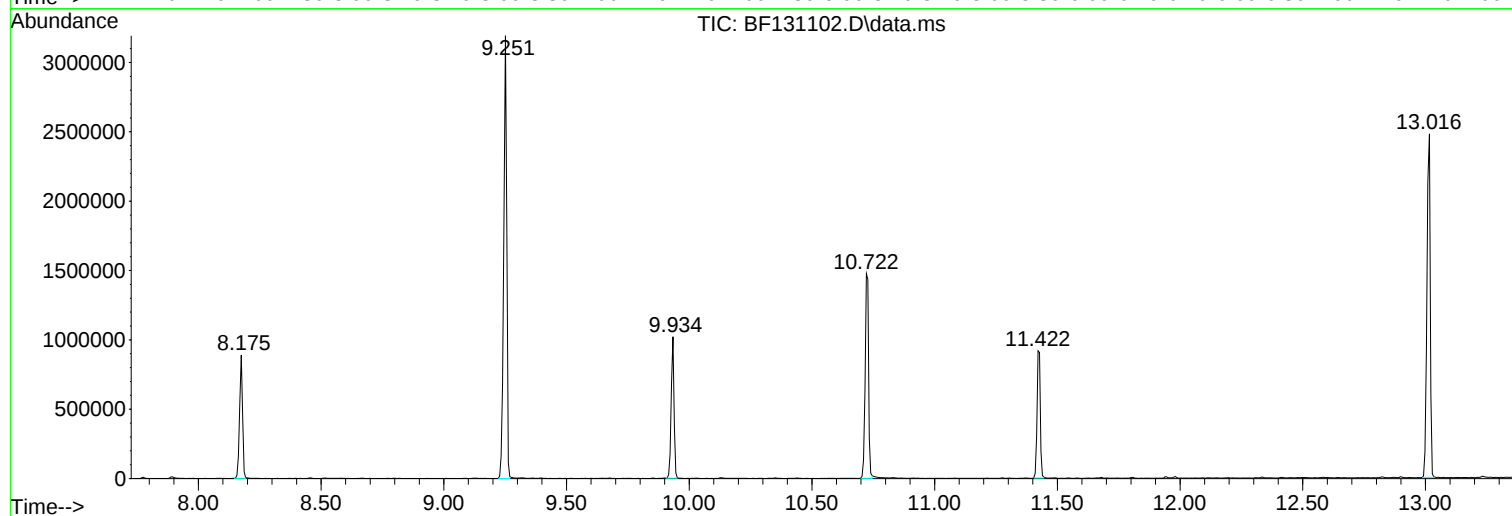
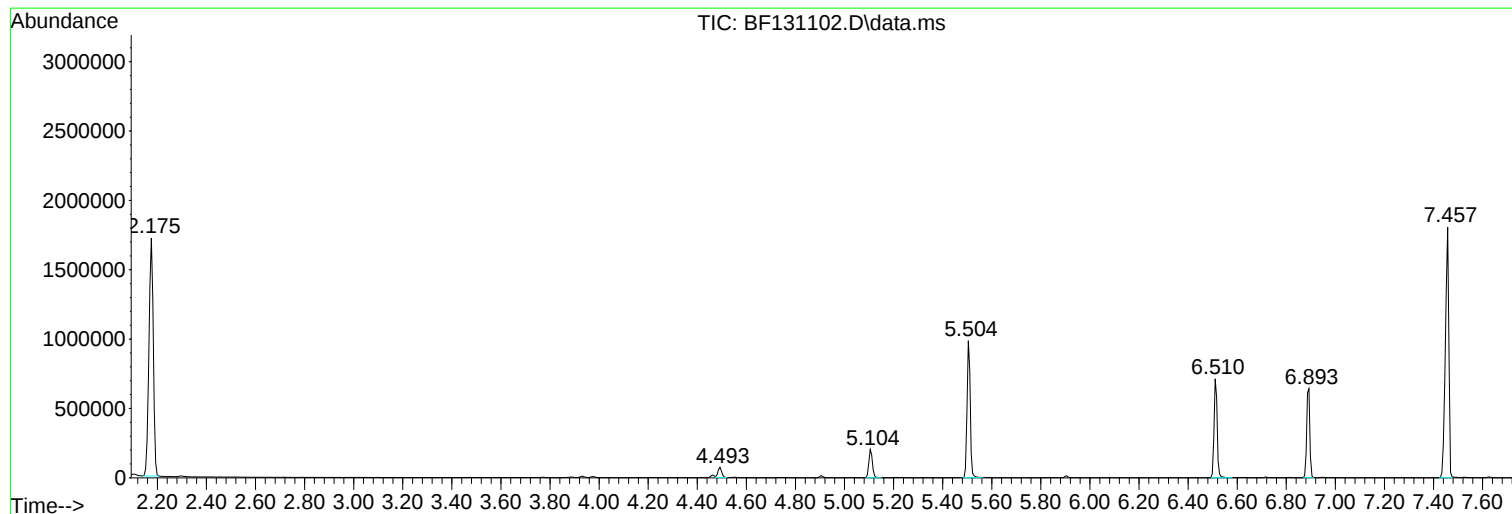
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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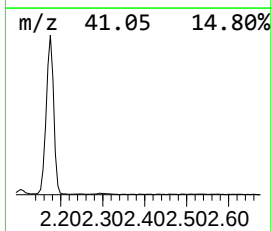
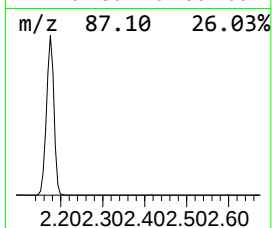
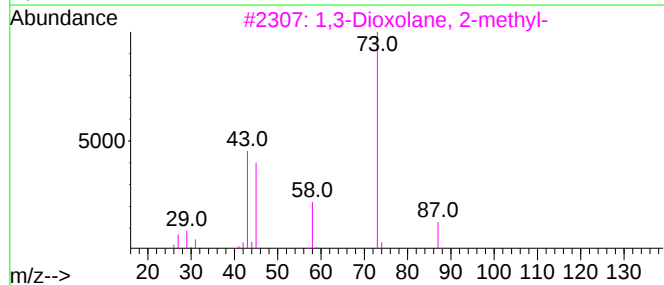
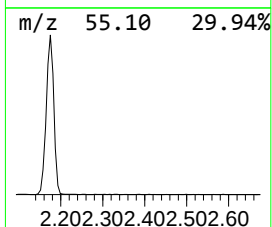
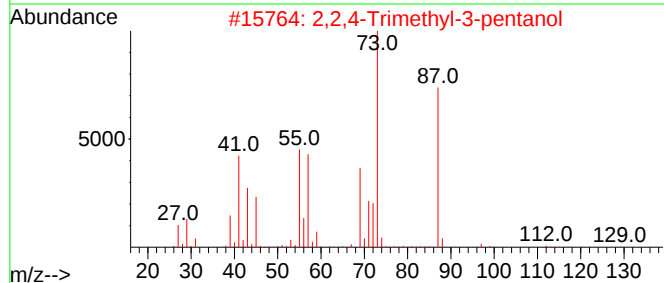
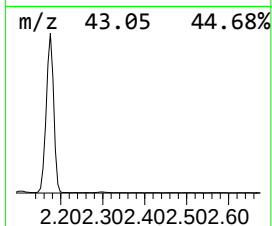
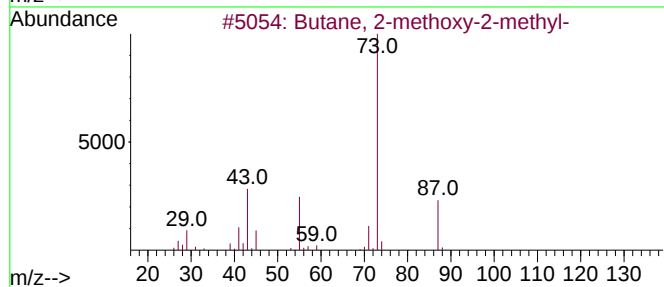
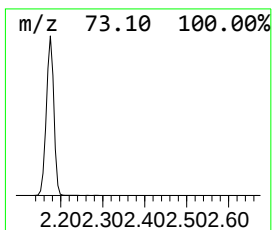
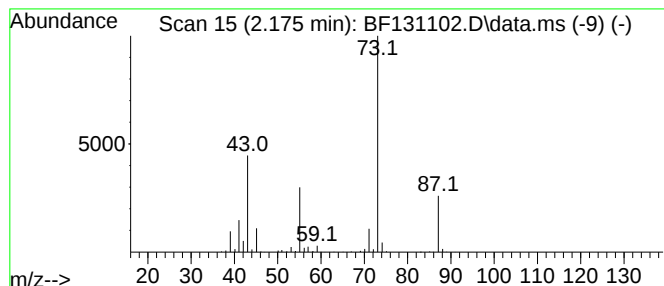
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	74.35 ng	2112420	1,4-Dichlorobenzene-d4	6.893

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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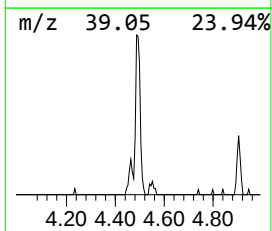
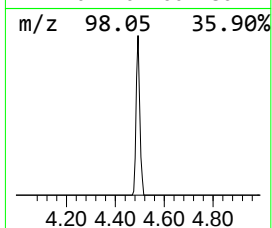
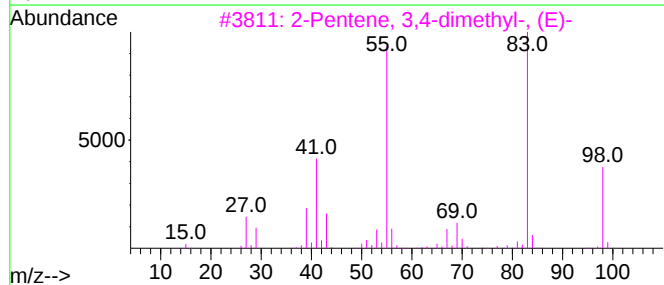
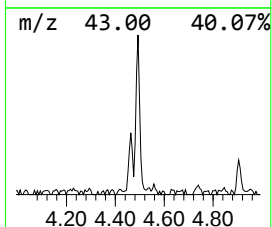
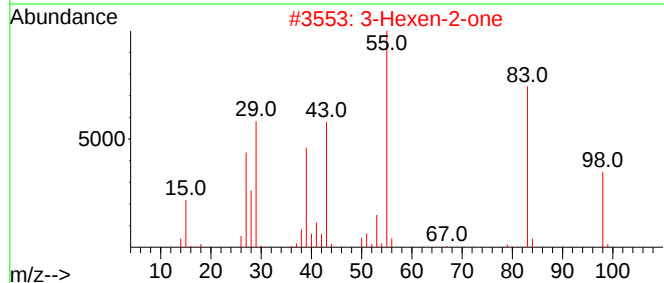
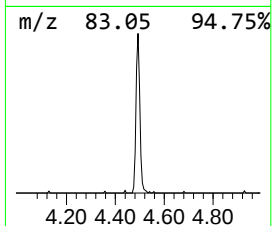
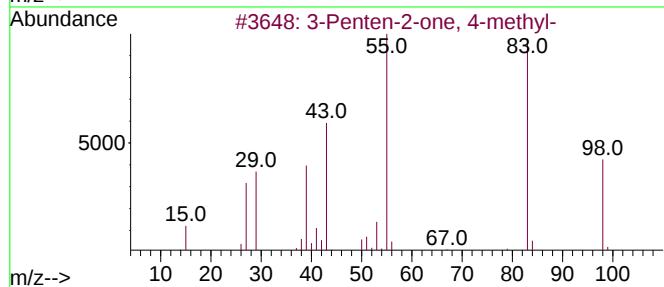
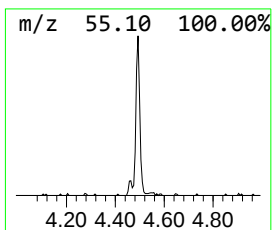
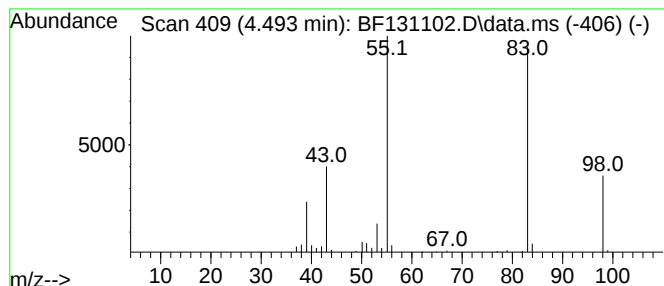
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.493	2.78 ng	78950	1,4-Dichlorobenzene-d4	6.893

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	72
5		2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	64



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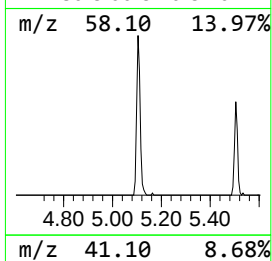
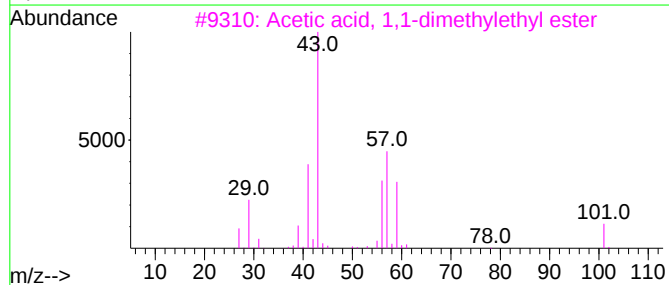
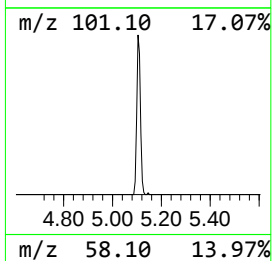
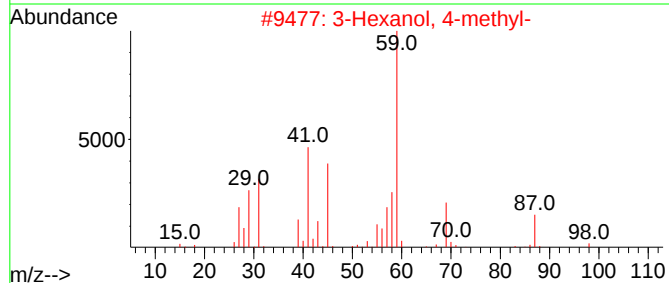
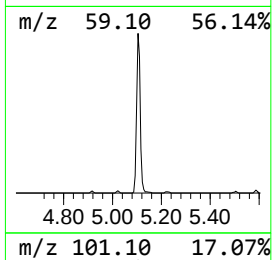
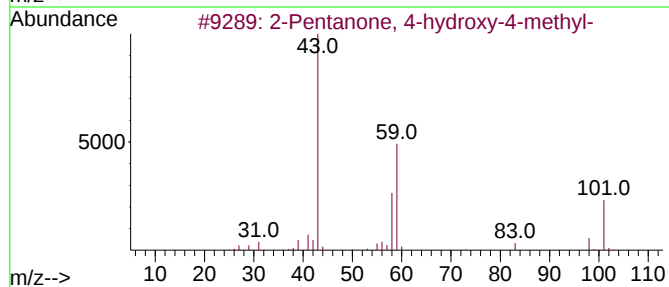
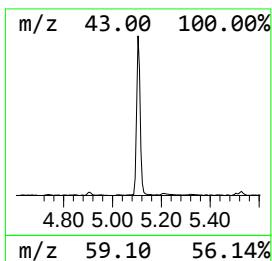
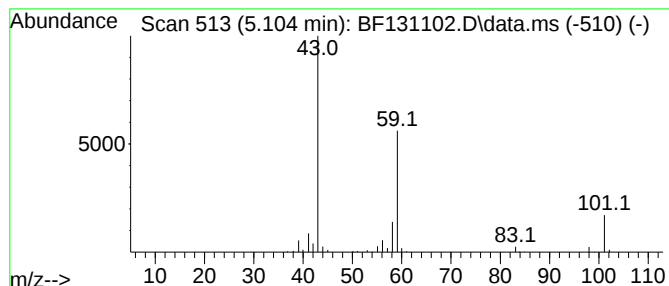
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	7.13 ng	202693	1,4-Dichlorobenzene-d4	6.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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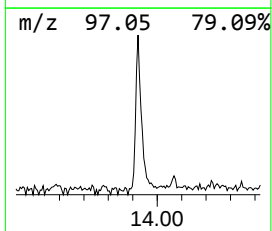
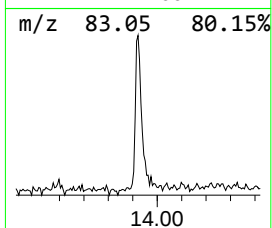
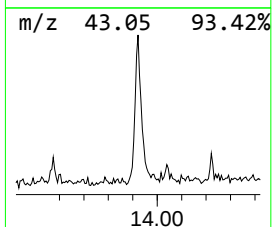
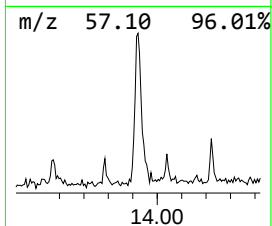
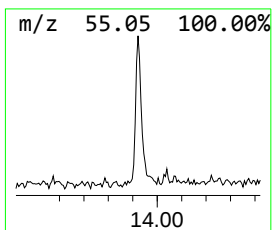
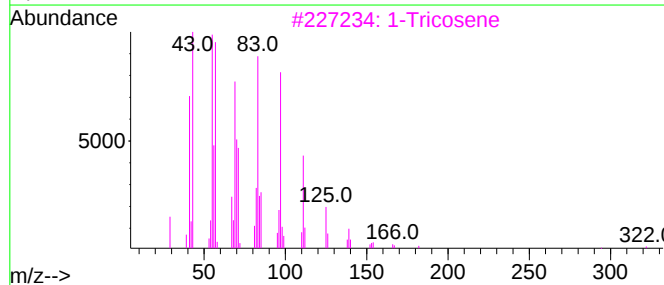
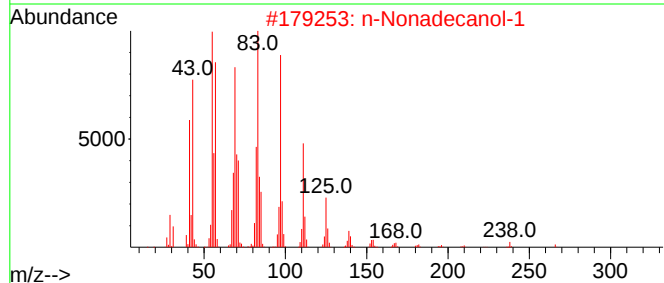
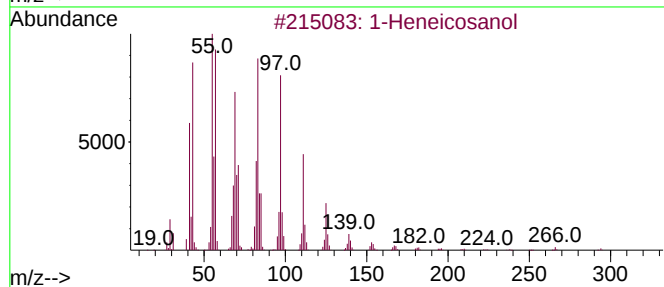
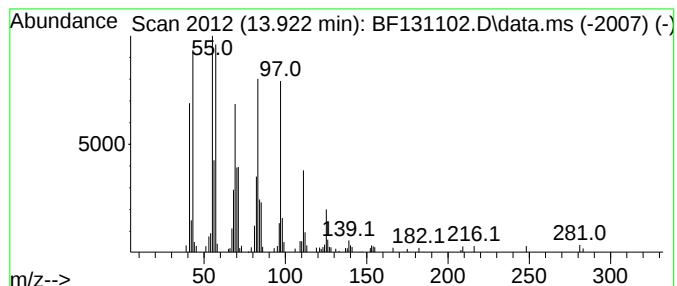
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.922	5.36 ng	164215	Chrysene-d12	14.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3			1-Tricosene	322	C23H46	018835-32-0	94
4			1-Nonadecene	266	C19H38	018435-45-5	91
5			1-Docosene	308	C22H44	001599-67-3	91



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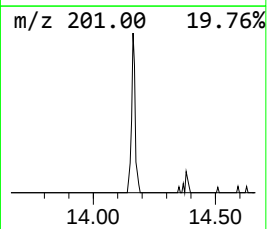
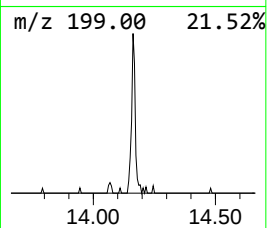
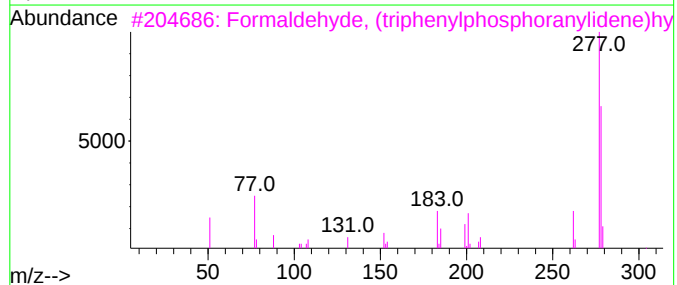
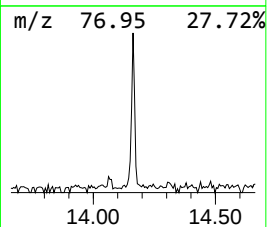
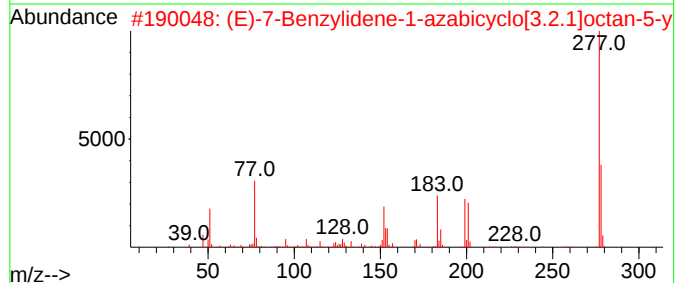
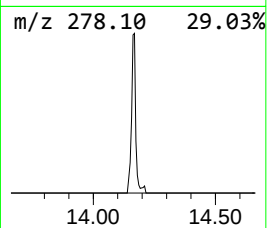
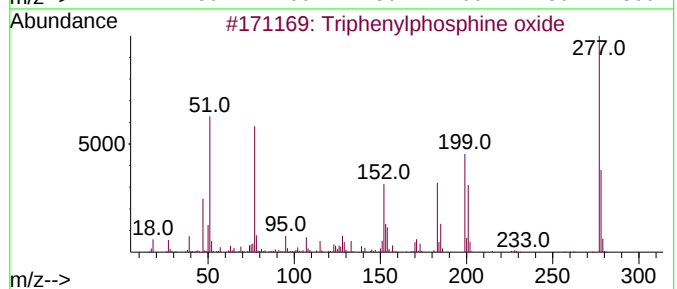
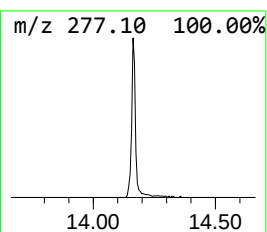
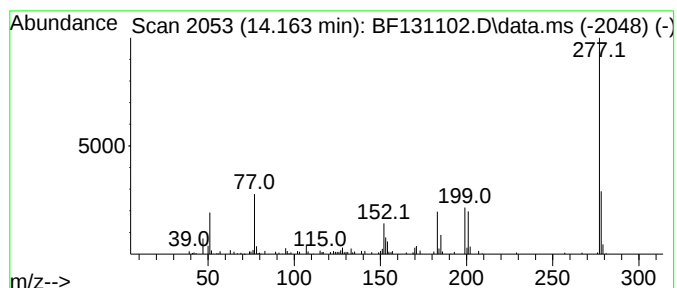
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.163	2.97 ng	91149	Chrysene-d12	14.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	90
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15N02	1000080-00-3	43
5			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	37



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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...	2.175	74.3	ng	2112420	1	6.893	568222	20.0
3-Penten-2-one,...	4.493	2.8	ng	78950	1	6.893	568222	20.0
2-Pentanone, 4-...	5.104	7.1	ng	202693	1	6.893	568222	20.0
1-Heneicosanol	13.922	5.4	ng	164215	5	14.069	613089	20.0
Triphenylphosph...	14.163	3.0	ng	91149	5	14.069	613089	20.0