

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020325\
 Data File : BF141385.D
 Acq On : 03 Feb 2025 22:37
 Operator : RC/JU
 Sample : Q1269-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-231

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-BF012925.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141385.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.763	108	114	123	rVB	245054	396100	10.43%	1.749%
2	4.593	414	425	432	rBV	78650	118388	3.12%	0.523%
3	4.663	432	437	443	rVB	60692	85129	2.24%	0.376%
4	5.040	495	501	509	rVB2	173797	272939	7.19%	1.205%
5	5.428	561	567	582	rBV	2143302	2902035	76.42%	12.813%
6	6.440	732	739	756	rBV	2023575	2887031	76.02%	12.747%
7	6.793	794	799	804	rBV	442273	535400	14.10%	2.364%
8	7.357	888	895	900	rBV	1528942	2101366	55.33%	9.278%
9	8.075	1011	1017	1022	rBV	535254	706301	18.60%	3.118%
10	9.151	1193	1200	1205	rBV	2652692	3710737	97.71%	16.384%
11	9.828	1309	1315	1320	rBV	624360	804936	21.20%	3.554%
12	10.622	1443	1450	1468	rBV	1747748	2412253	63.52%	10.651%
13	11.316	1562	1568	1575	rBV	650357	809593	21.32%	3.575%
14	11.845	1653	1658	1673	rBV2	53869	98914	2.60%	0.437%
15	12.910	1832	1839	1844	rBV	2782944	3797603	100.00%	16.767%
16	13.957	2011	2017	2026	rBV	436838	585212	15.41%	2.584%
17	15.404	2257	2263	2275	rBV	269109	425029	11.19%	1.877%

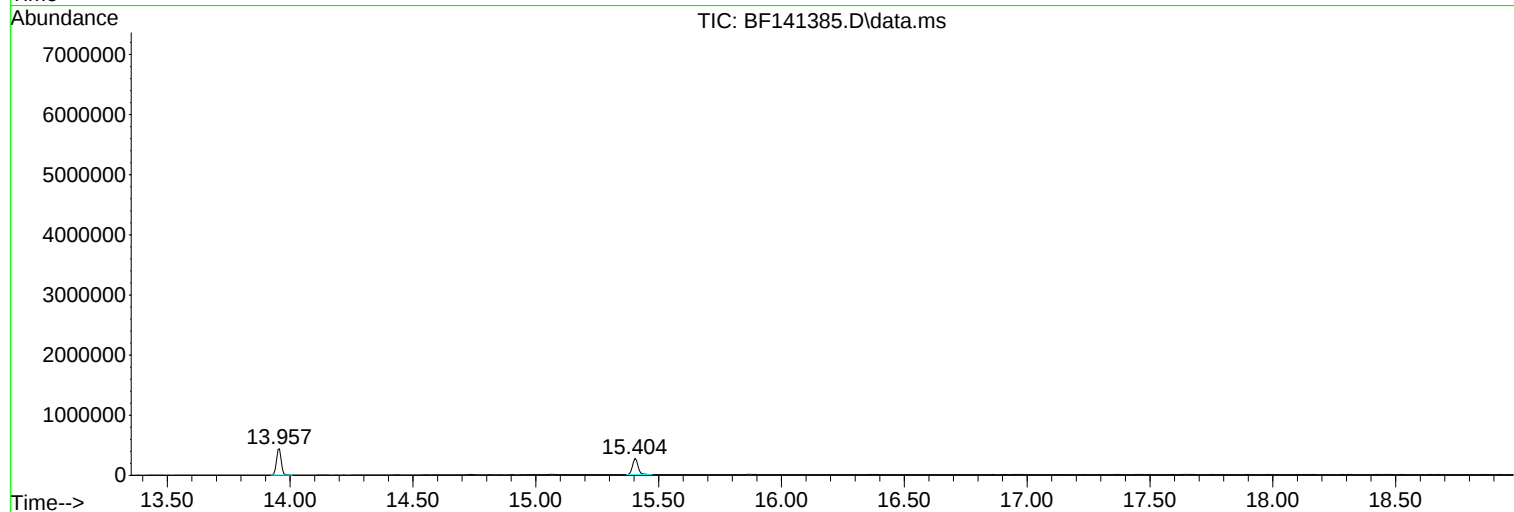
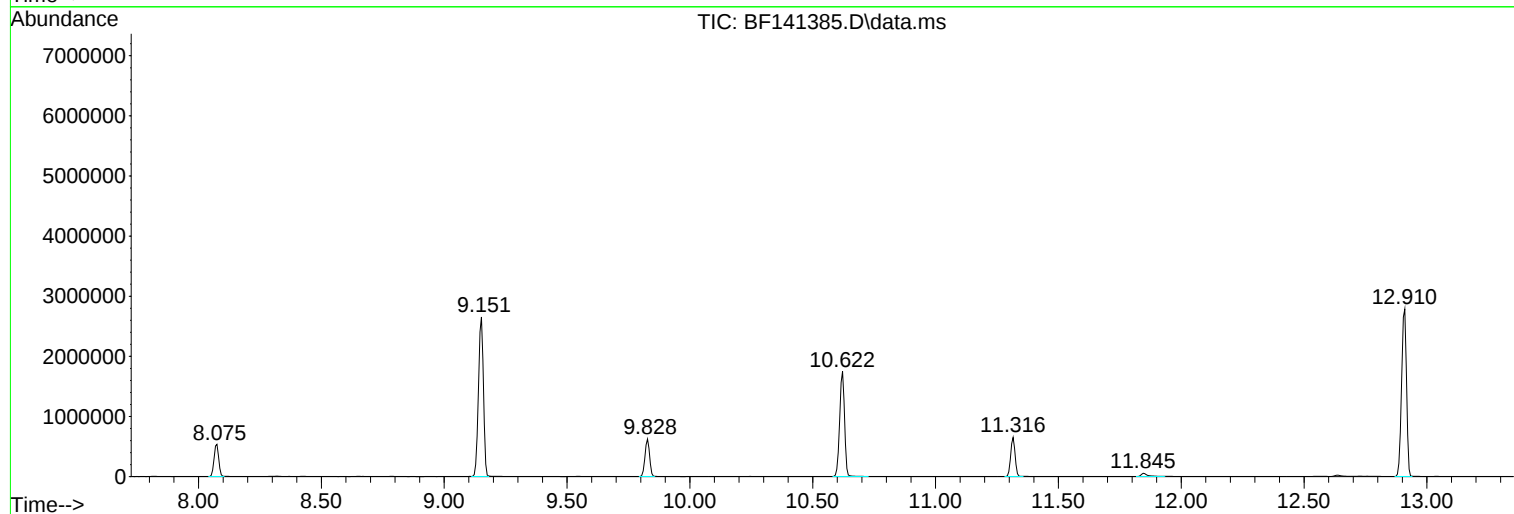
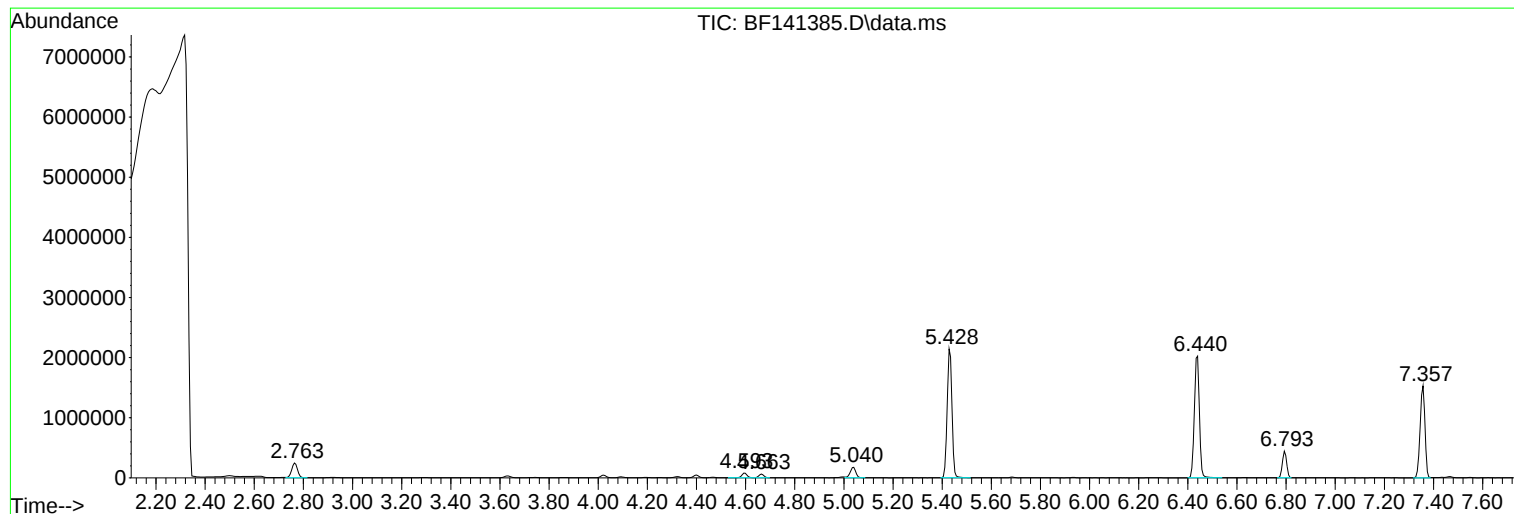
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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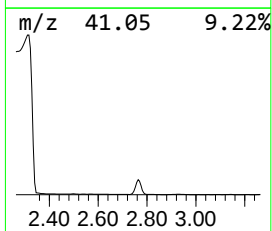
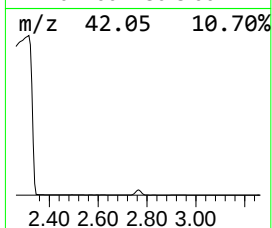
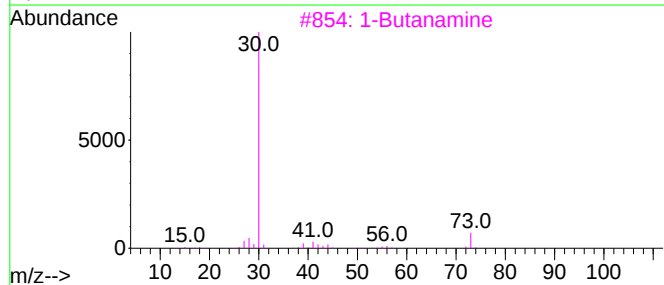
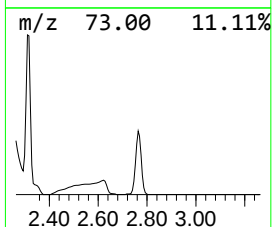
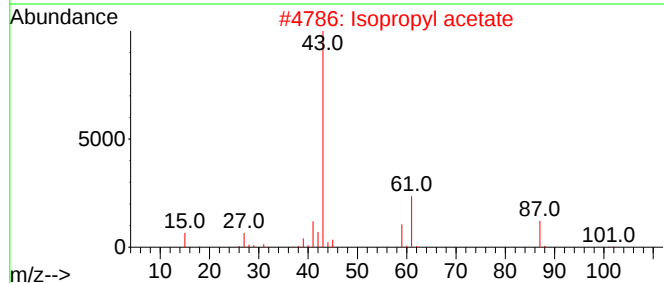
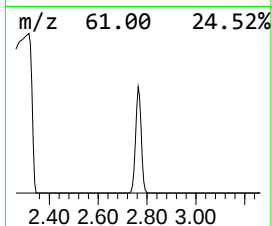
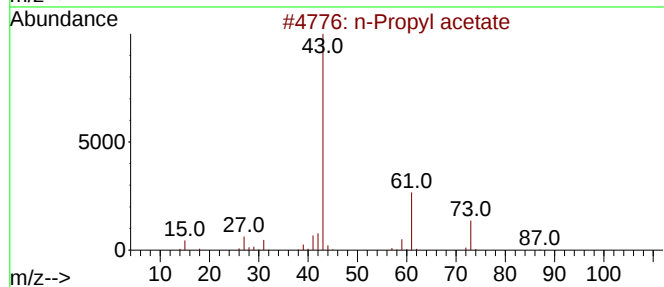
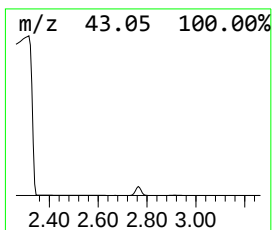
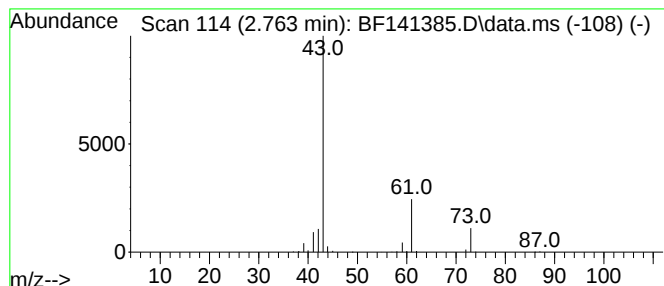
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF012925.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.763	14.80 ng	396100	1,4-Dichlorobenzene-d4	6.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	83
2			Isopropyl acetate	102	C5H10O2	000108-21-4	38
3			1-Butanamine	73	C4H11N	000109-73-9	5
4			Isobutylamine	73	C4H11N	000078-81-9	5
5			Ethanimidic acid, ethyl ester	87	C4H9NO	001000-84-6	4



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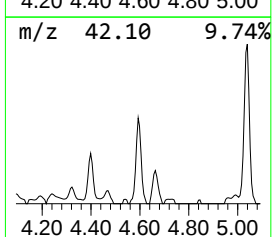
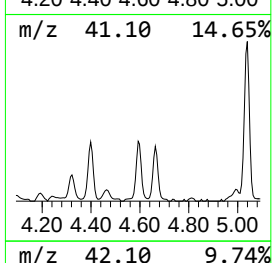
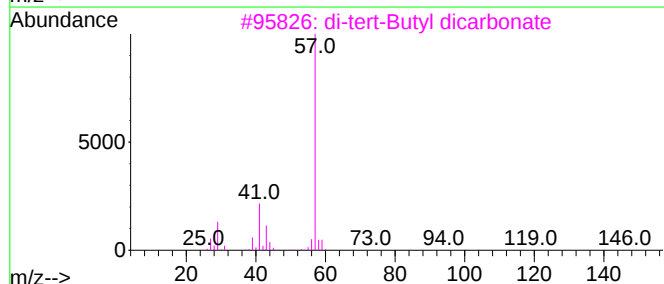
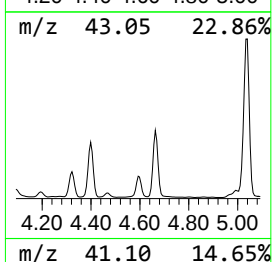
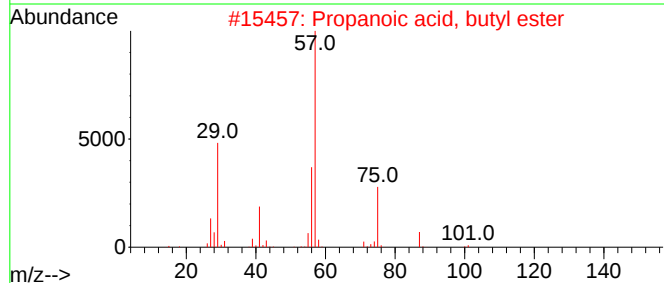
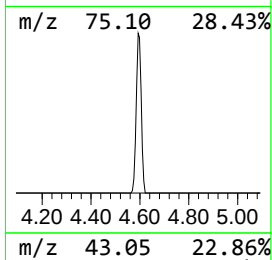
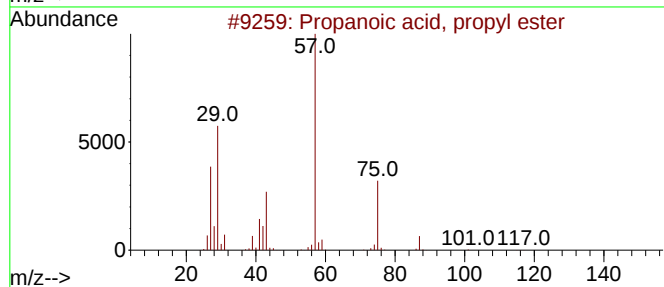
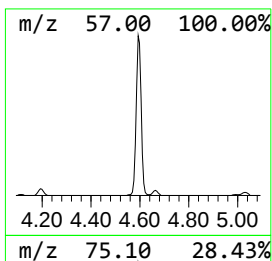
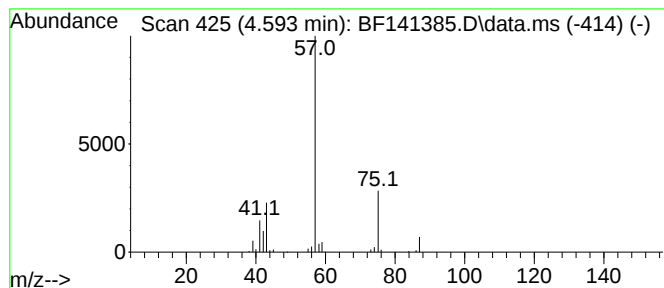
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.593	4.42 ng	118388	1,4-Dichlorobenzene-d4	6.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	36
3			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	16
4			Azetidine	57	C3H7N	000503-29-7	9
5			Propanoic acid, anhydride	130	C6H10O3	000123-62-6	9



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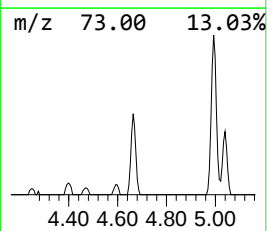
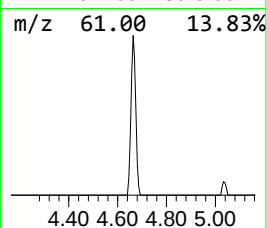
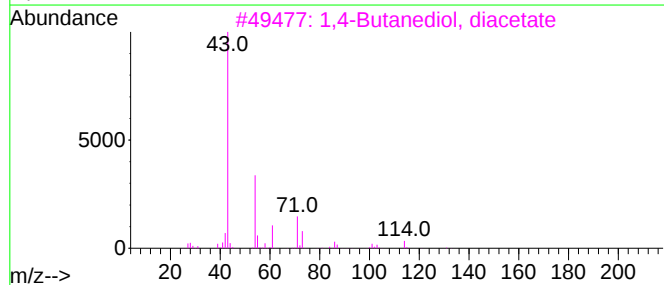
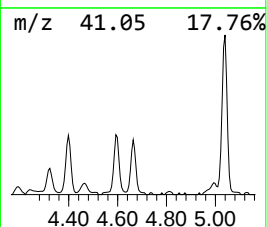
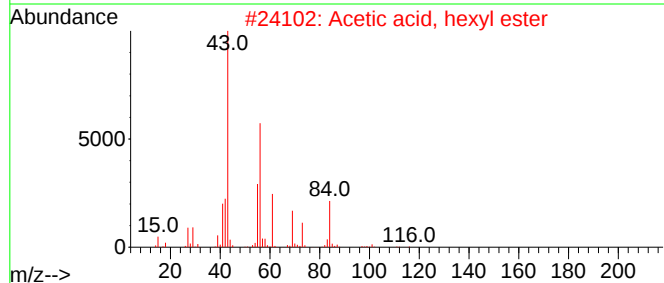
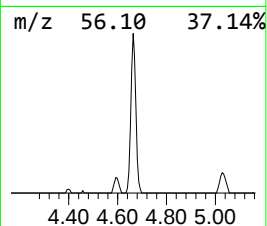
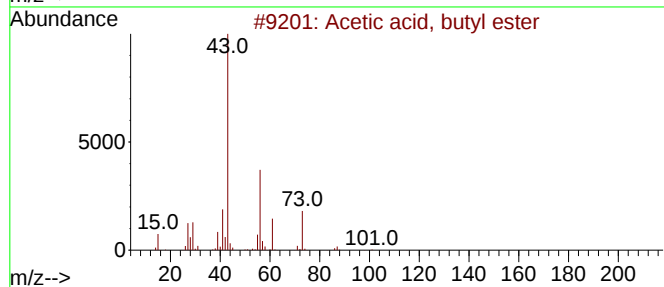
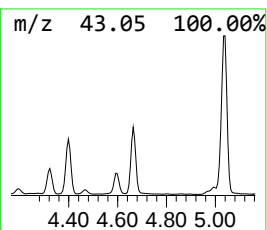
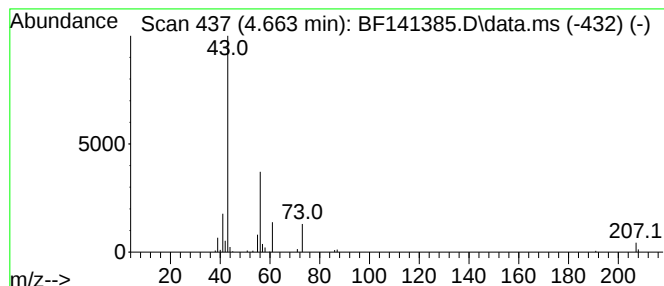
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Peak Number 3 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.663	3.18 ng	85129	1,4-Dichlorobenzene-d4	6.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	33
3			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	25
4			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	25
5			Di-n-propyl ether	102	C6H14O	000111-43-3	17



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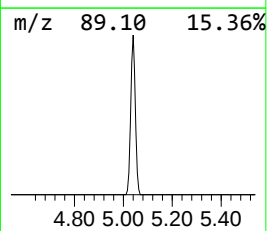
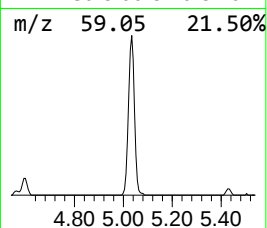
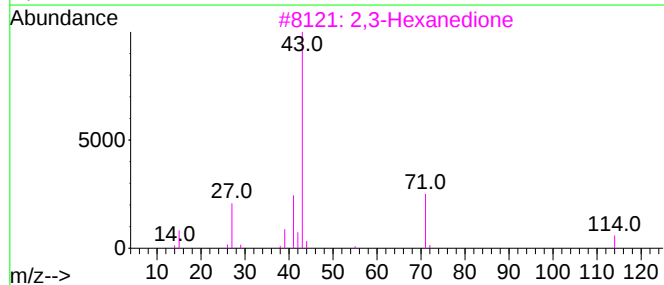
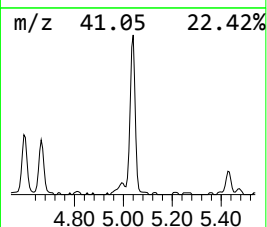
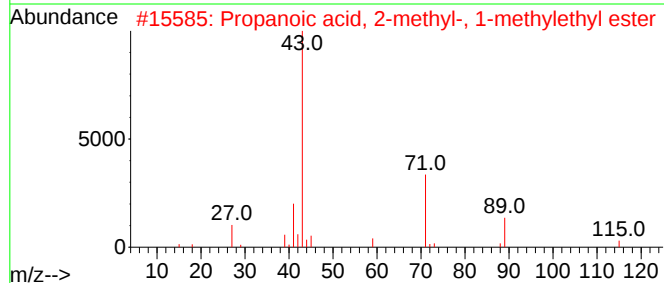
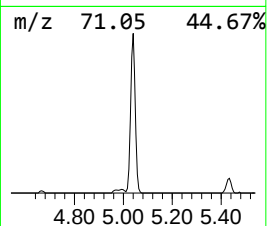
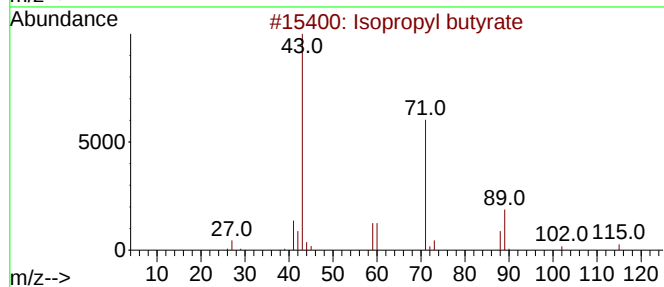
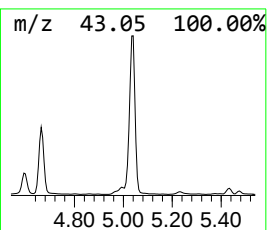
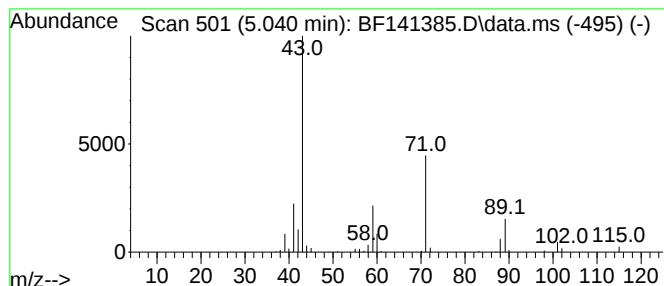
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Peak Number 4 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	10.20 ng	272939	1,4-Dichlorobenzene-d4	6.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	64
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
3			2,3-Hexanedione	114	C6H10O2	003848-24-6	47
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	42
5			Butanoic acid, 2-ethyl-, methyl ...	130	C7H14O2	000816-11-5	39



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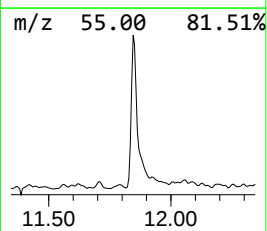
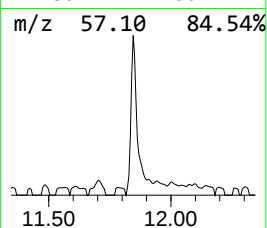
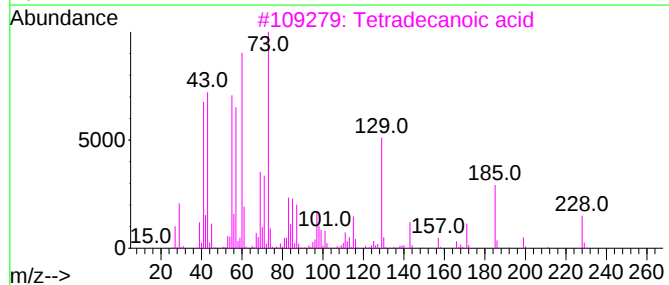
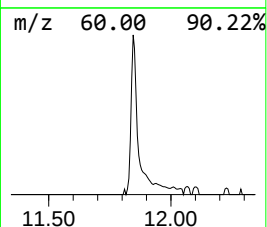
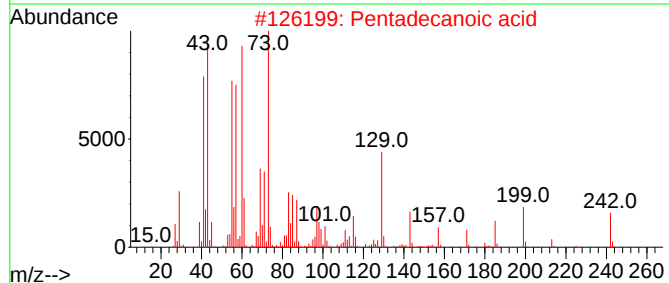
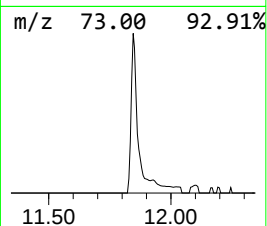
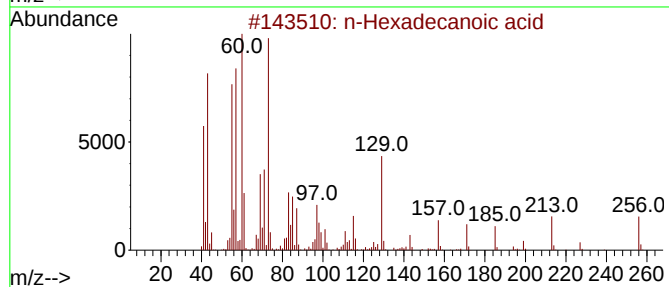
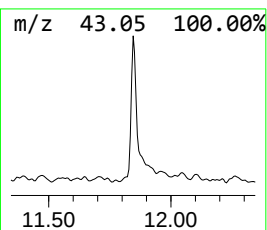
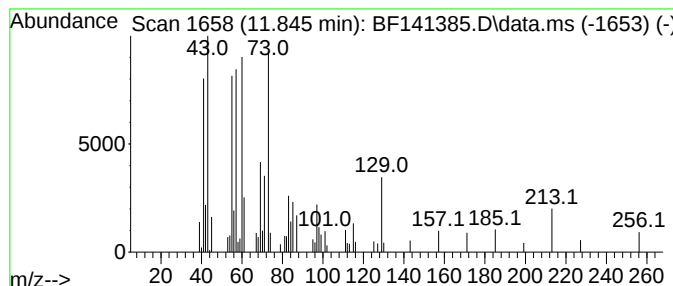
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TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	2.44 ng	98914	Phenanthrene-d10	11.316

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.763	14.8	ng	396100	1	6.793	535400	20.0
Propanoic acid,...	4.593	4.4	ng	118388	1	6.793	535400	20.0
Acetic acid, bu...	4.663	3.2	ng	85129	1	6.793	535400	20.0
Isopropyl butyrate	5.040	10.2	ng	272939	1	6.793	535400	20.0
n-Hexadecanoic ...	11.845	2.4	ng	98914	4	11.316	809593	20.0