LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM073123\
Data File : BM041202.D
Acq On : 01 Aug 2023 00:14
Operator : MA/JU
Sample : 03741-12
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
B-P6A

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_M\Methods\8270-BM072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041202.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	364	371	383	rBV	1913903	2713667	50.43%	7.665%
2	6.975	637	644	662	rBV	1736667	2802197	52.07%	7.915%
3	7.798	777	784	792	rBV	716285	1092822	20.31%	3.087%
4	8.975	976	984	999	rBV	1087849	1772539	32.94%	5.007%
5	10.604	1255	1261	1281	rVB	869818	1445751	26.87%	4.084%
6	10.757	1281	1287	1298	rBV2	28256	71224	1.32%	0.201%
7	11.845	1459	1472	1484	rBV	196369	354339	6.58%	1.001%
8	13.080	1672	1682	1694	rBV	2709944	3861986	71.76%	10.909%
9	13.927	1819	1826	1838	rBV	137373	203924	3.79%	0.576%
10	14.463	1911	1917	1926	rBV	1227542	1724414	32.04%	4.871%
11	15.962	2164	2172	2181	rBV	2159492	2966962	55.13%	8.381%
12	17.221	2380	2386	2392	rBV	1466251	2007995	37.31%	5.672%
13	18.121	2534	2539	2549	rBV	284243	473873	8.81%	1.339%
14	19.286	2730	2737	2744	rBV	104016	201668	3.75%	0.570%
15	19.403	2754	2757	2768	rBV3	86426	157998	2.94%	0.446%
16	19.650	2796	2799	2808	rVB2	115241	182668	3.39%	0.516%
17	19.856	2829	2834	2847	rBV	4500124	5381498	100.00%	15.201%
18	21.133	3047	3051	3060	rVB2	265350	404222	7.51%	1.142%
19	21.421	3095	3100	3105	rBV	1855141	2326647	43.23%	6.572%
20	21.833	3167	3170	3179	rVB2	176160	287328	5.34%	0.812%
21	22.015	3197	3201	3206	rVB	2381917	2720512	50.55%	7.685%
22	23.791	3497	3503	3511	rVB	1206376	2247291	41.76%	6.348%

Sum of corrected areas: 35401525

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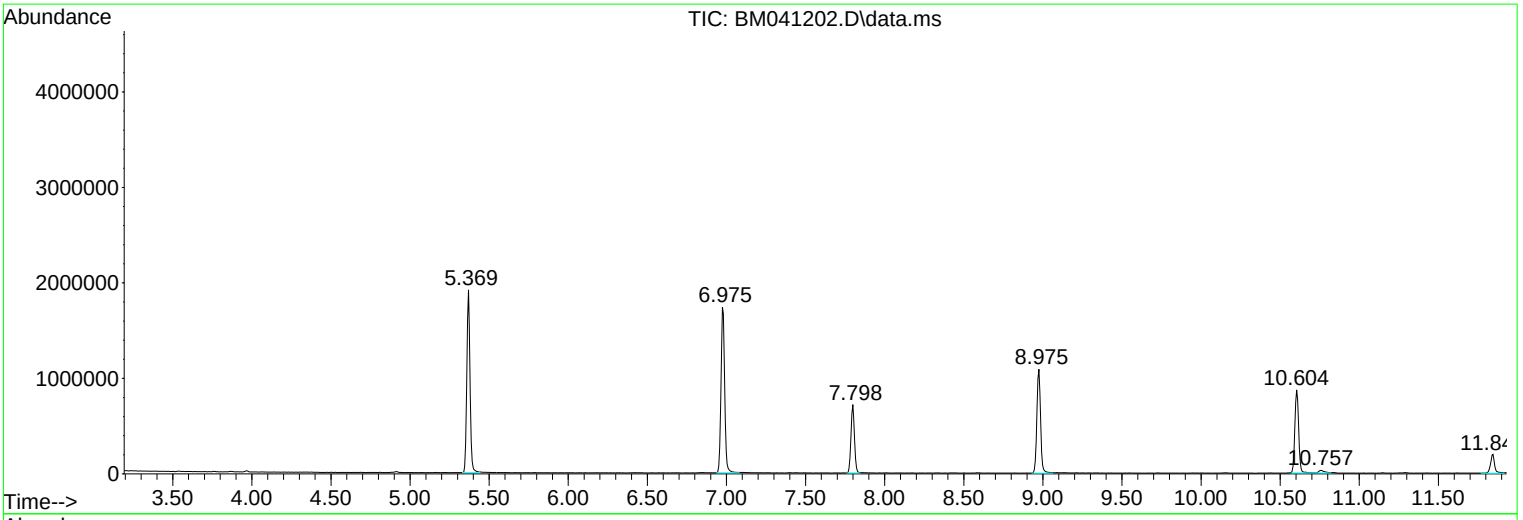
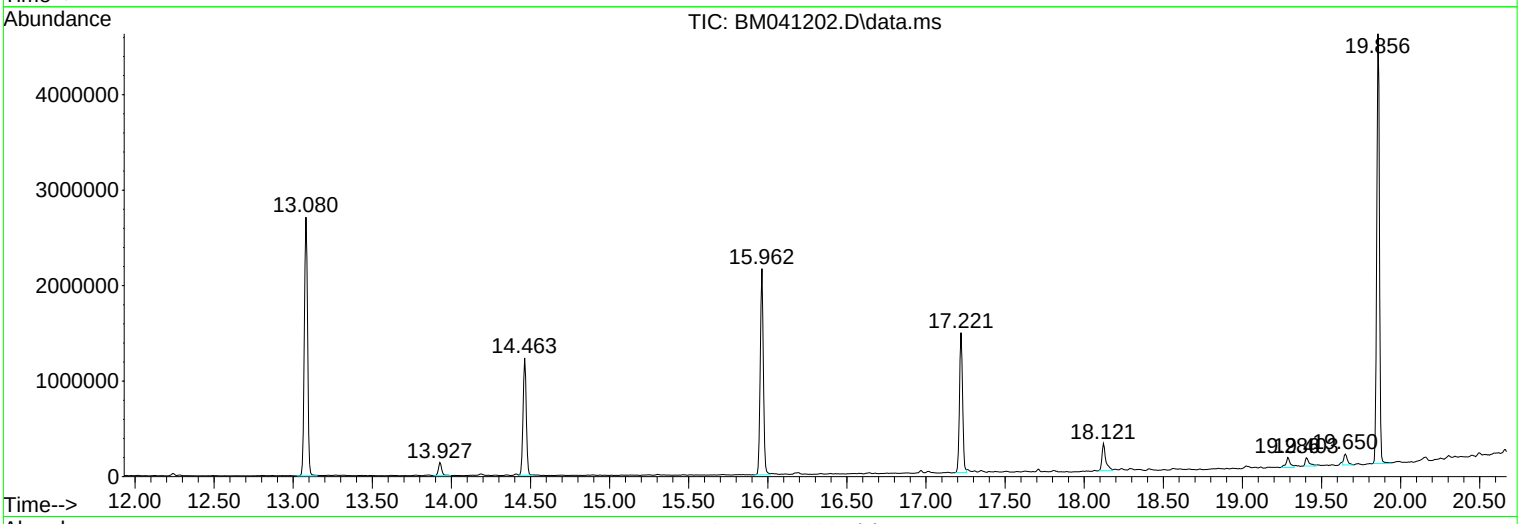
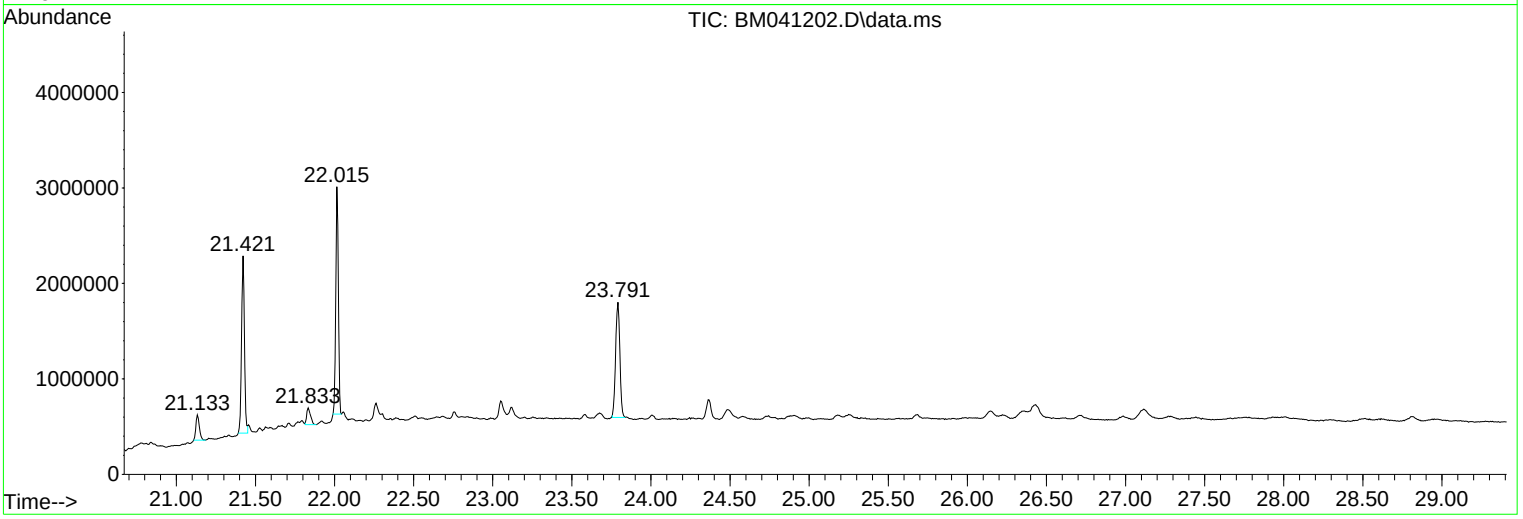
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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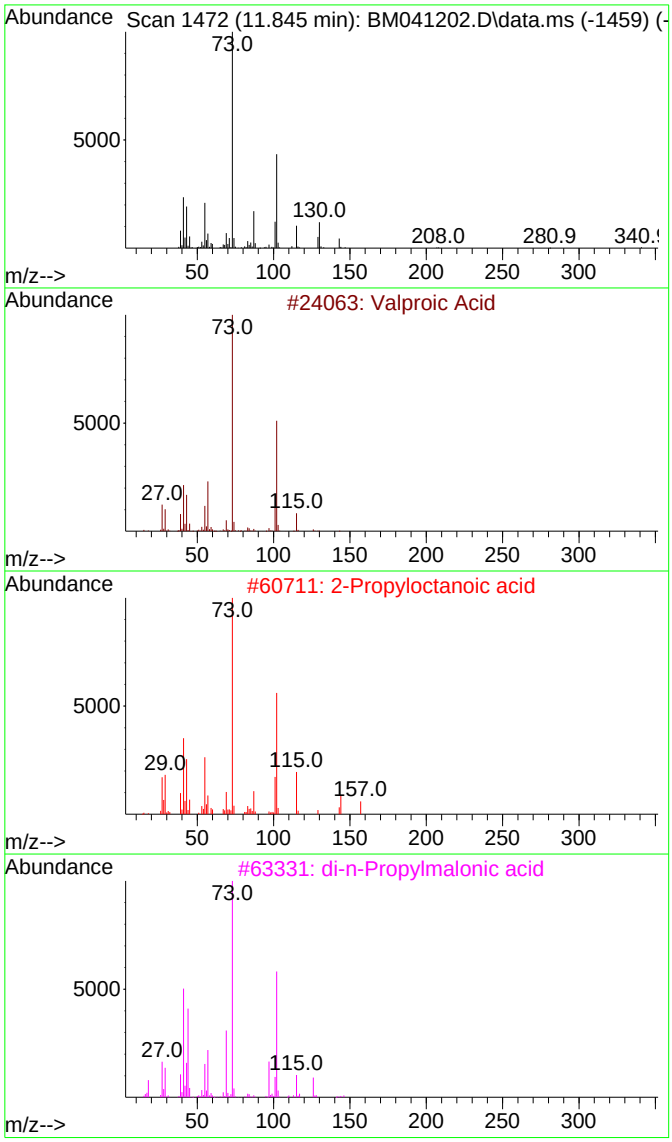
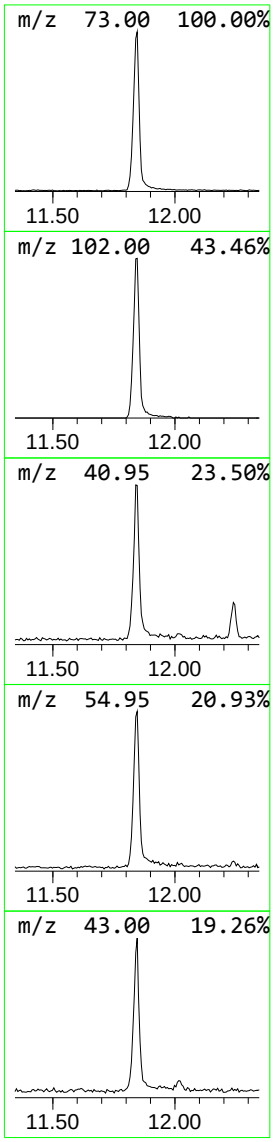
Peak Number 1 Valproic Acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	4.90 ng	354339	Naphthalene-d8	10.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Valproic Acid	144	C8H16O2	000099-66-1	53
2	2-Propyloctanoic acid	186	C11H22O2	031080-41-8	42
3	di-n-Propylmalonic acid	188	C9H16O4	001636-27-7	42
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	16
5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	10





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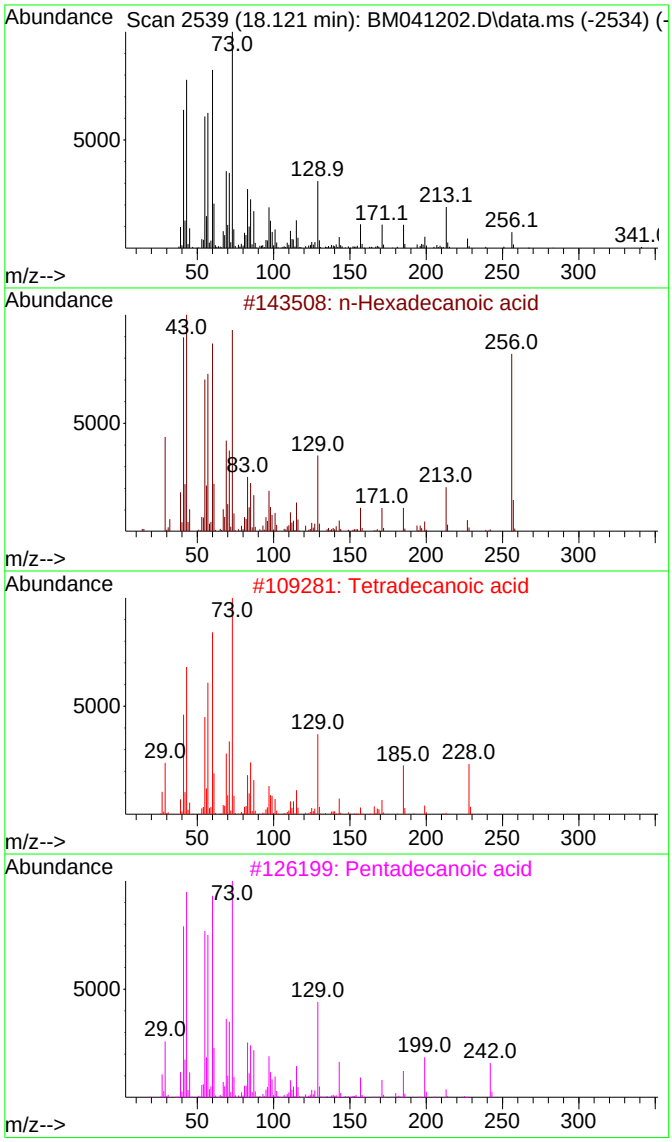
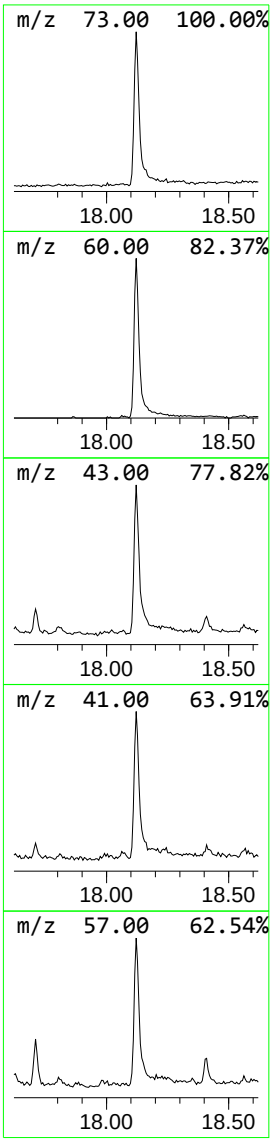
Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.121	4.72 ng	473873	Phenanthrene-d10	17.221

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	87





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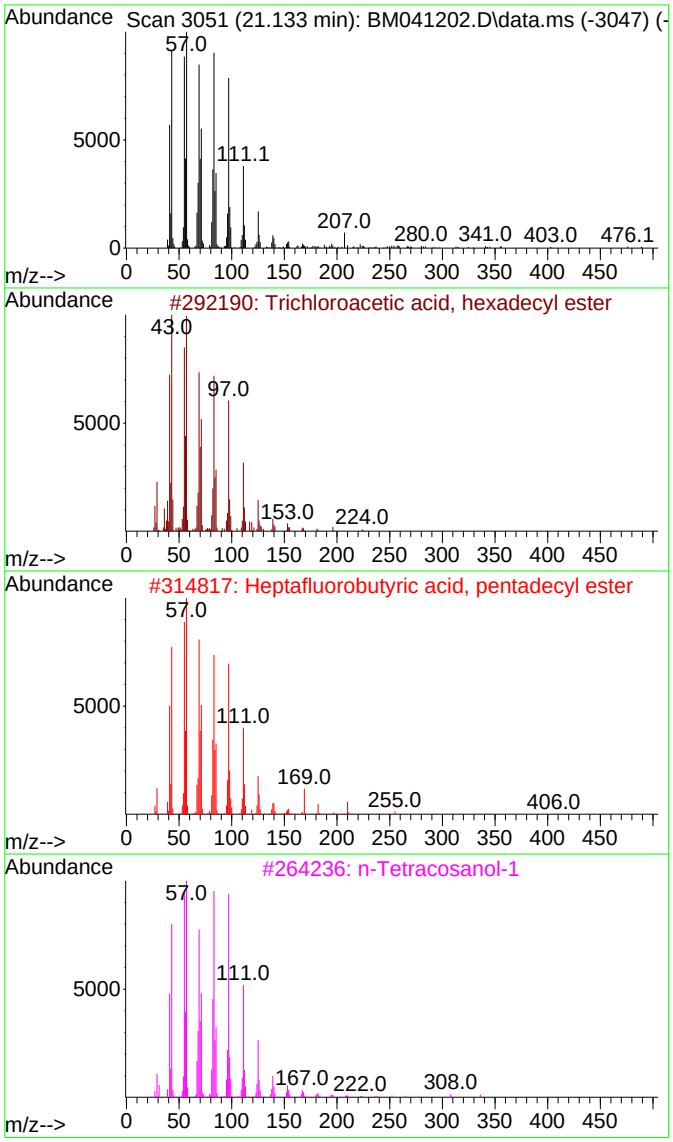
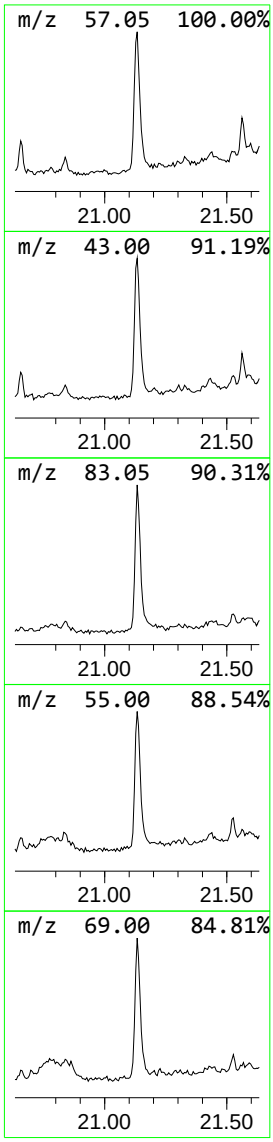
Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	3.47 ng	404222	Chrysene-d12	21.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94





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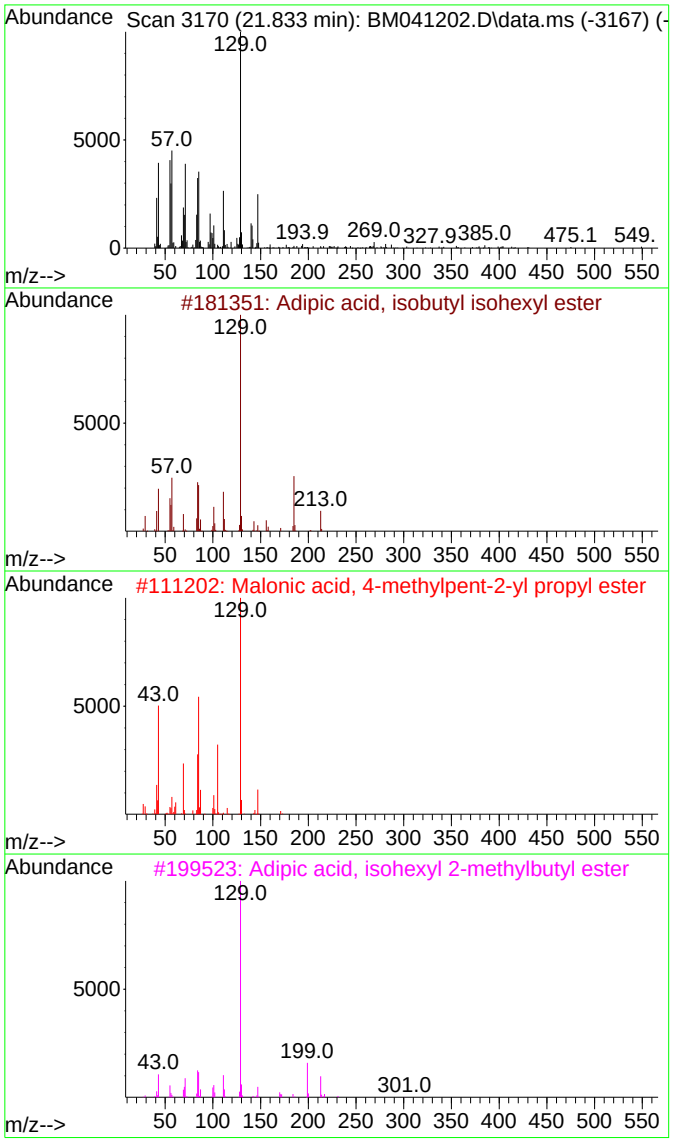
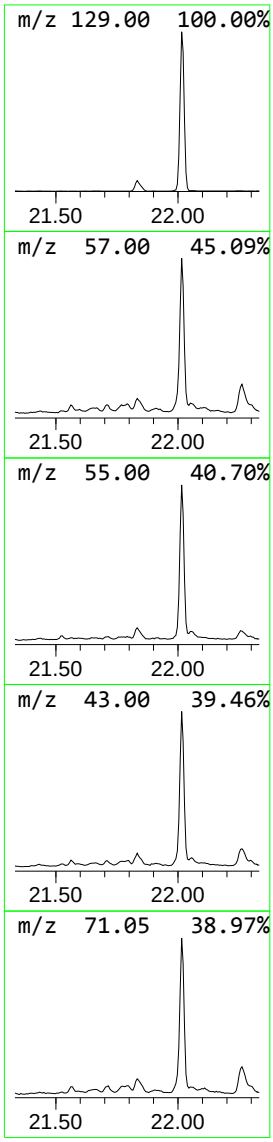
Peak Number 5 unknown21.833 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.833	2.47 ng	287328	Chrysene-d12	21.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, isobutyl isohexyl e...	286	C16H30O4	1000324-09-5	47
2	Malonic acid, 4-methylpent-2-yl ...	230	C12H22O4	1000349-33-1	43
3	Adipic acid, isohexyl 2-methylbu...	300	C17H32O4	1000324-67-4	38
4	Succinic acid, 3,3-dimethylbut-2...	230	C12H22O4	1000349-50-5	35
5	2-Heptenoic acid, undecyl ester	282	C18H34O2	1010406-09-6	35





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
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TIC Library : C:\Database\NIST20.L
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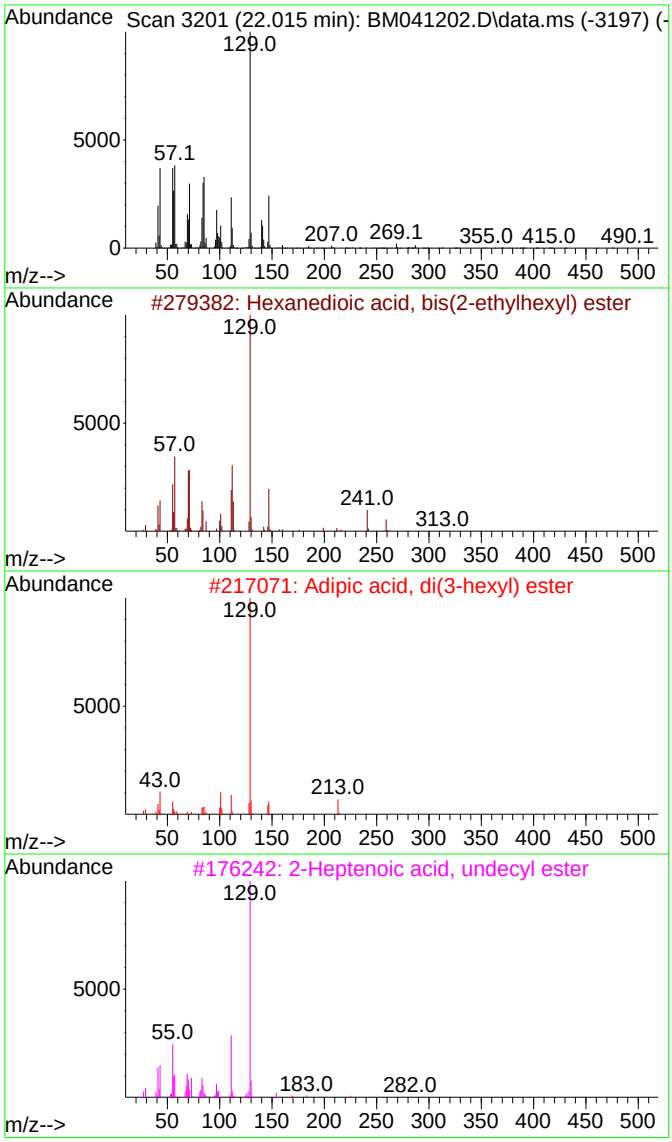
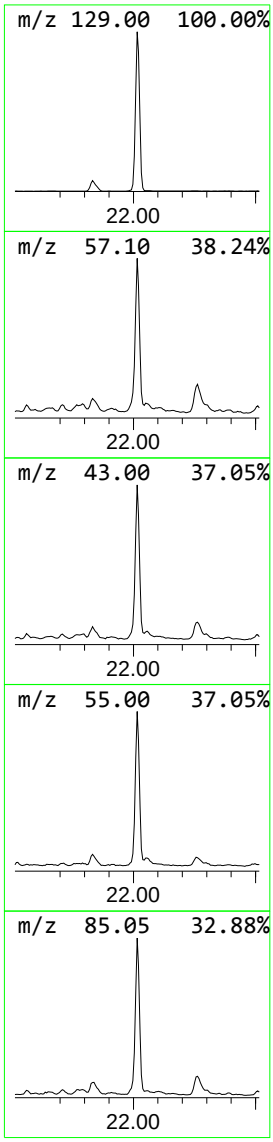
****
Peak Number 6 Hexanedioic acid, bis(2-eth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.015	23.39 ng	2720510	Chrysene-d12	21.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	52
2	Adipic acid, di(3-hexyl) ester	314	C18H34O4	1000353-63-9	47
3	2-Heptenoic acid, undecyl ester	282	C18H34O2	1010406-09-6	43
4	Adipic acid, isohexyl 3-pentyl e...	300	C17H32O4	1000324-60-7	43
5	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	43





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Valproic Acid	11.845	4.9	ng	354339	2	10.604	1445750	20.0
n-Hexadecanoic ...	18.121	4.7	ng	473873	4	17.221	2008000	20.0
Trichloroacetic...	21.133	3.5	ng	404222	5	21.421	2326650	20.0
unknown21.833	21.833	2.5	ng	287328	5	21.421	2326650	20.0
Hexanedioic aci...	22.015	23.4	ng	2720510	5	21.421	2326650	20.0