LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071921\
Data File : BF124617.D
Acq On : 19 Jul 2021 17:02
Operator : JU/CG
Sample : M3076-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210578-COM-1

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-BF070721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124617.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.246	24	27	32	rBB	13353	16523	6.56%	1.027%
2	5.157	519	522	526	rBB	2588	2980	1.18%	0.185%
3	5.534	581	586	589	rBB	187761	186036	73.81%	11.565%
4	6.534	750	756	759	rBV	167951	192617	76.42%	11.974%
5	6.910	818	820	823	rBB	43954	36500	14.48%	2.269%
6	7.475	911	916	919	rBB	125797	126357	50.13%	7.855%
7	8.092	1018	1021	1024	rBV	33823	27704	10.99%	1.722%
8	8.198	1035	1039	1042	rBB	59601	51826	20.56%	3.222%
9	9.275	1217	1222	1225	rBB	277064	252059	100.00%	15.670%
10	9.957	1334	1338	1341	rBB	69861	62314	24.72%	3.874%
11	10.745	1467	1472	1475	rBB	191013	164799	65.38%	10.245%
12	11.186	1544	1547	1551	rBB	8257	8136	3.23%	0.506%
13	11.445	1587	1591	1594	rBV	80194	66230	26.28%	4.117%
14	11.968	1674	1680	1684	rBV	39513	38130	15.13%	2.370%
15	12.751	1809	1813	1817	rBB	20372	16745	6.64%	1.041%
16	13.033	1856	1861	1864	rBV	274259	241464	95.80%	15.011%
17	13.562	1947	1951	1955	rBB	42064	39809	15.79%	2.475%
18	13.939	2012	2015	2019	rBV3	4485	6785	2.69%	0.422%
19	14.080	2036	2039	2042	rBV	46852	40440	16.04%	2.514%
20	15.574	2288	2293	2297	rBB2	27131	31129	12.35%	1.935%

Sum of corrected areas: 1608583

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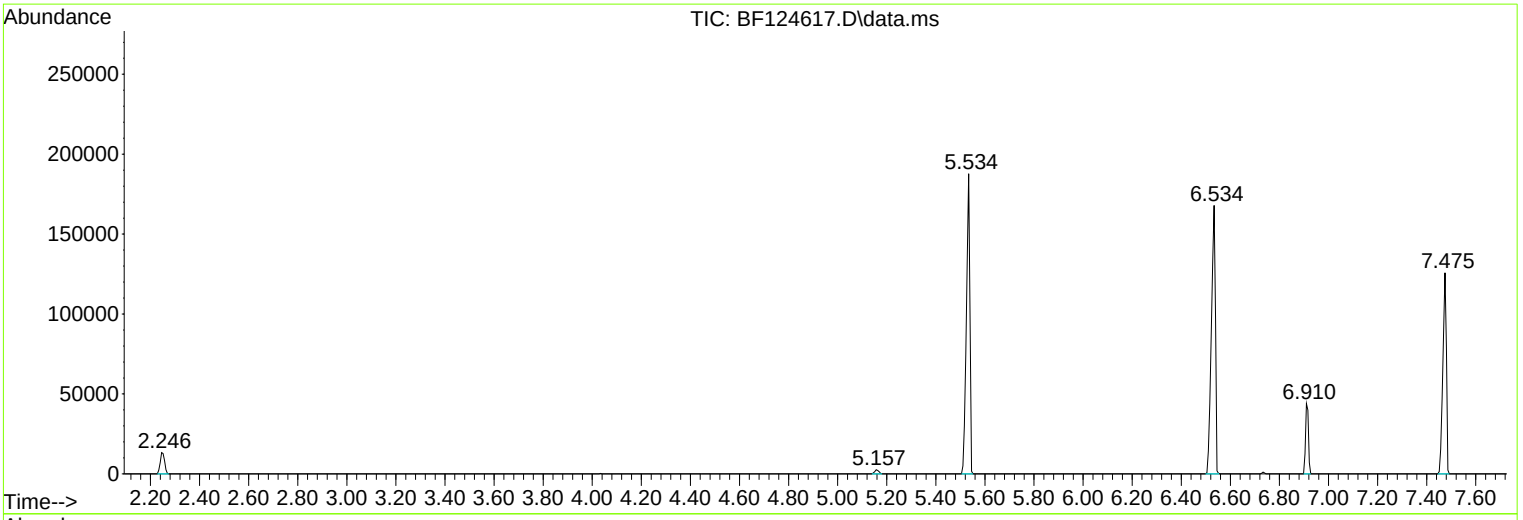
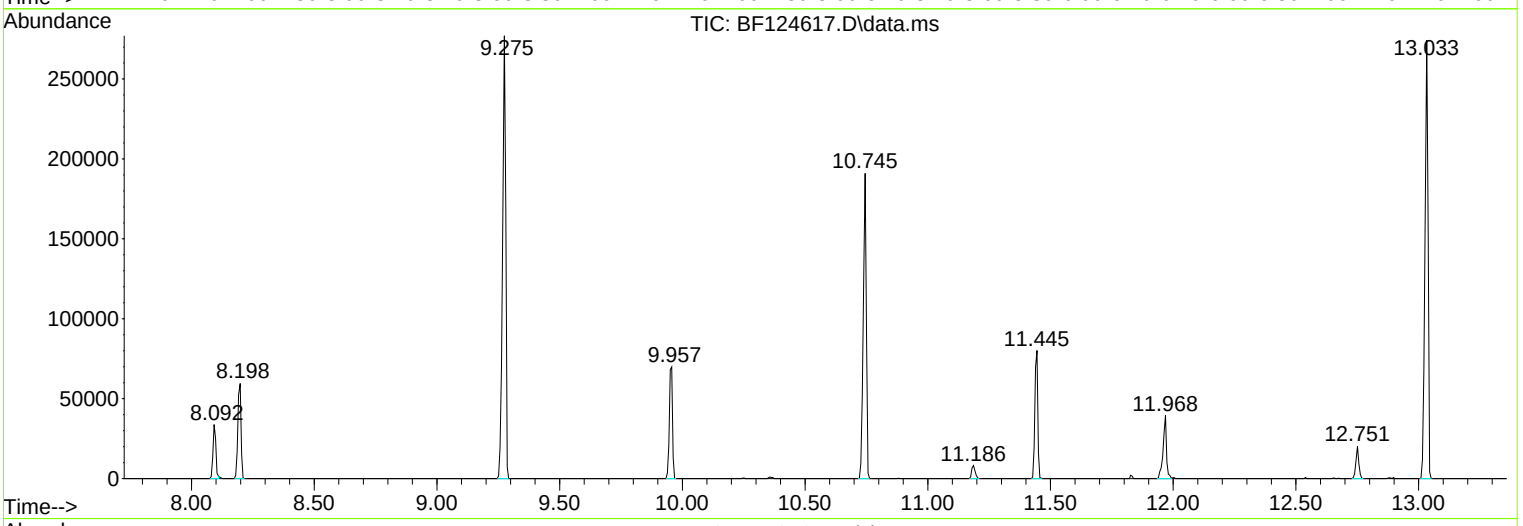
Misc :
ALS Vial : 11 Sample Multiplier: 1

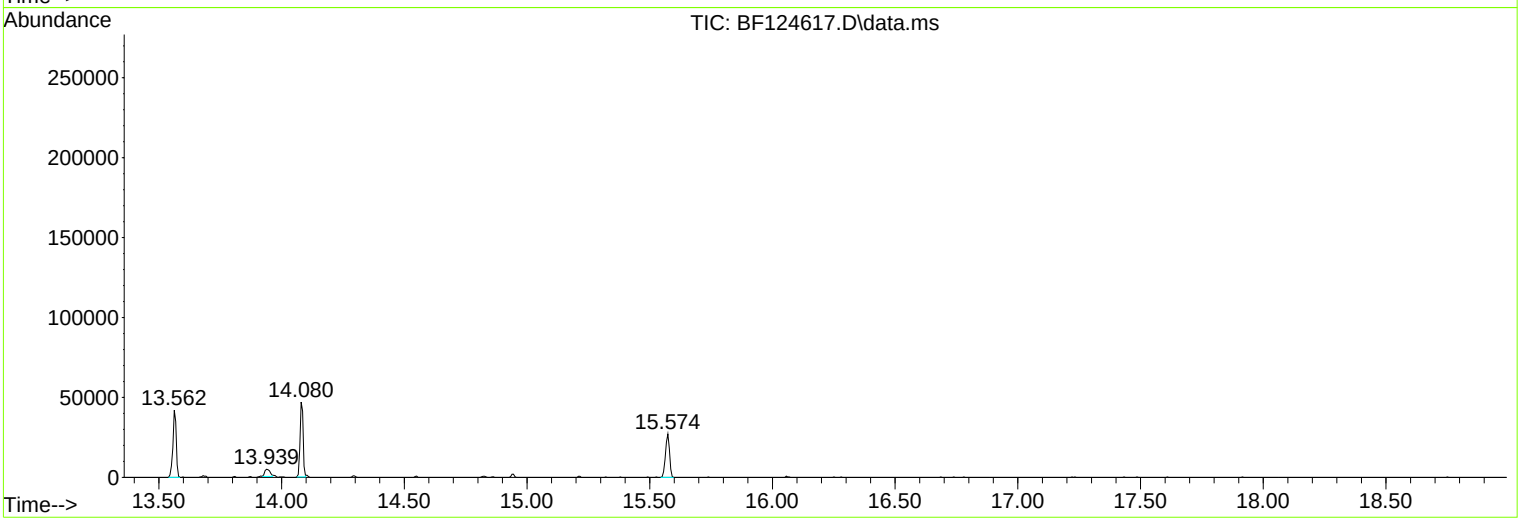
Instrument :
BNA_F
ClientSampleId :
20210578-COM-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.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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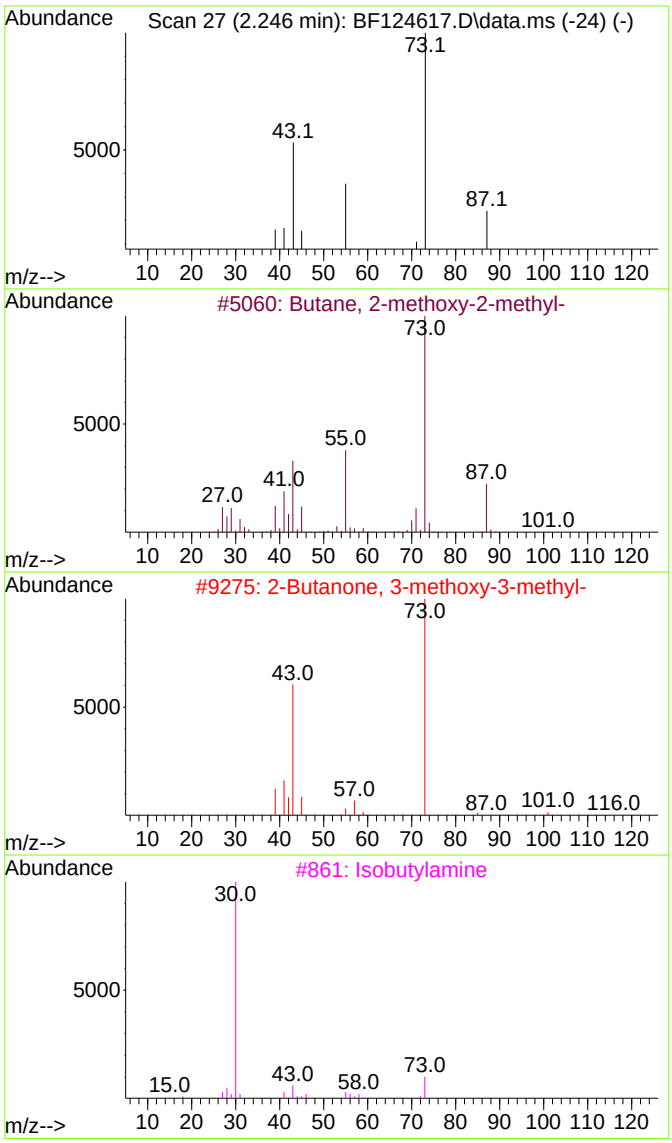
TIC Integration Parameters: LSCINT.P

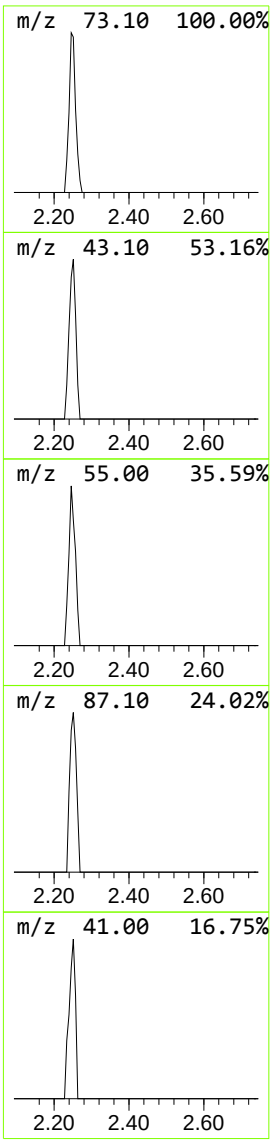
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.246	9.05 ng	16523	1,4-Dichlorobenzene-d4	6.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
3	Isobutylamine	73	C4H11N	000078-81-9	5
4	1-Pentanamine	87	C5H13N	000110-58-7	4
5	4-Ethoxy-2-butanone	116	C6H12O2	060044-74-8	4





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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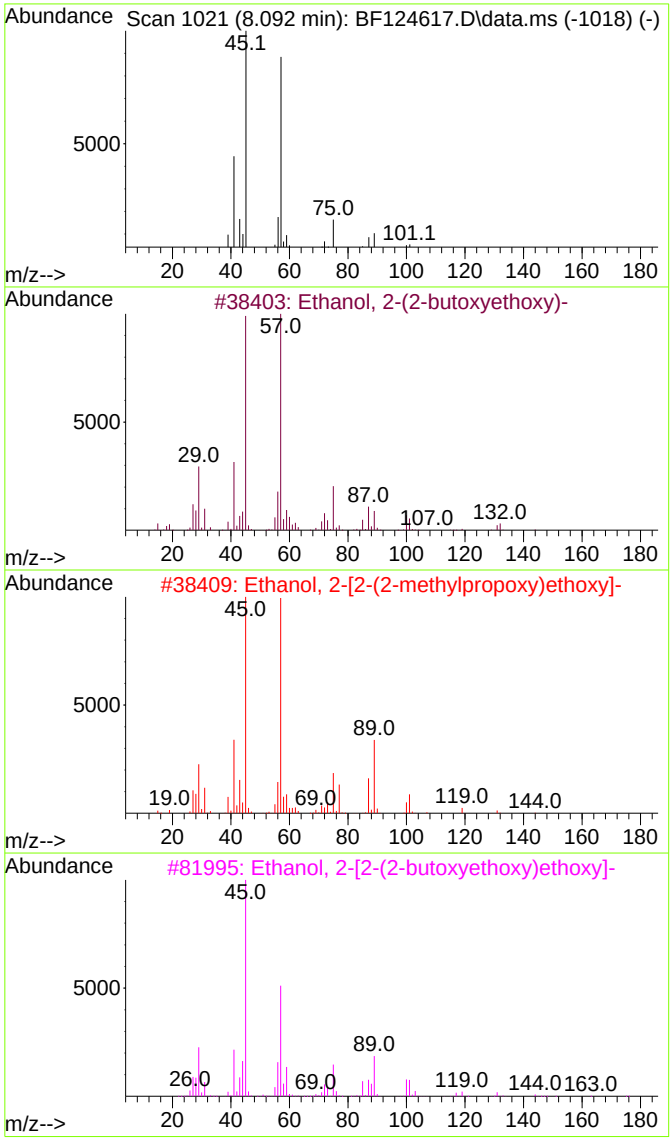
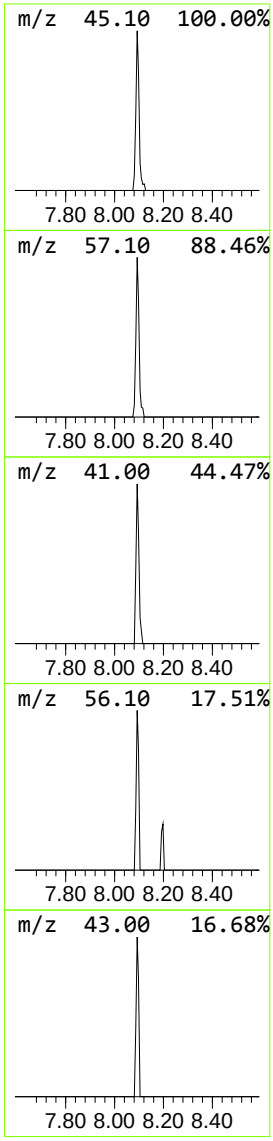
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	10.69 ng	27704	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, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4	Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	40
5	Oxirane, (ethoxymethyl)-	102	C5H10O2	004016-11-9	36





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Acq On : 19 Jul 2021 17:02
Operator : JU/CG
Sample : M3076-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20210578-COM-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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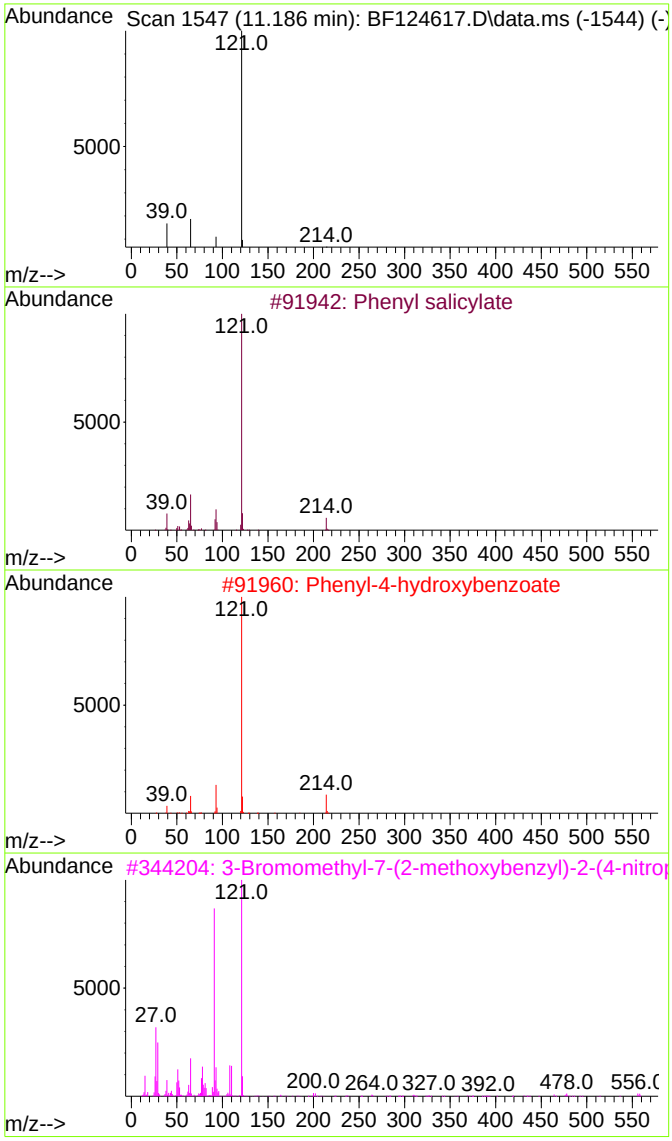
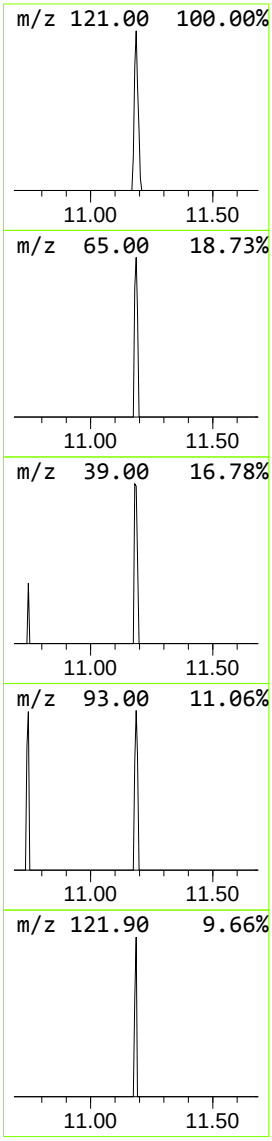
Peak Number 3 Phenyl salicylate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.186	2.46 ng	8136	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenyl salicylate	214	C13H10O3	000118-55-8	83
2	Phenyl-4-hydroxybenzoate	214	C13H10O3	017696-62-7	74
3	3-Bromomethyl-7-(2-methoxybenzyl...	556	C25H21BrN2O6S	174069-57-9	9
4	2-Hydroxy-N'-(prop-2-enoyl)benzo...	206	C10H10N2O3	1031422-82-8	9
5	3,5-Bis(4-hydroxybenzoyl)-1,2,4-...	326	C16H10N2O6	1000326-36-5	9





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Operator : JU/CG
Sample : M3076-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210578-COM-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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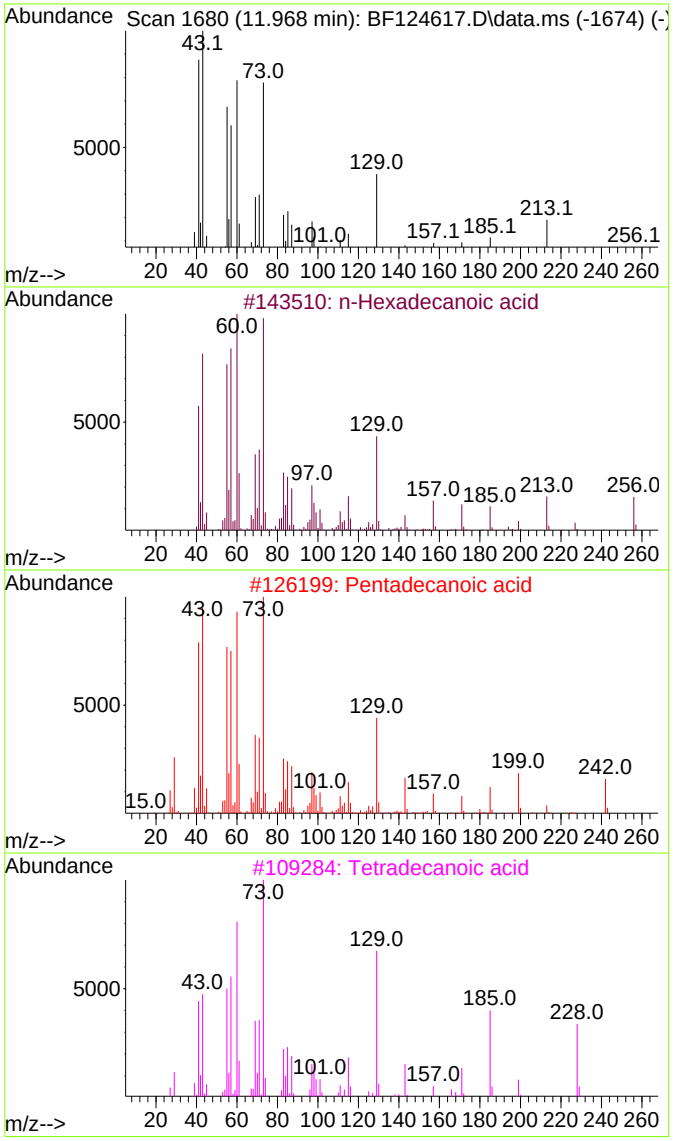
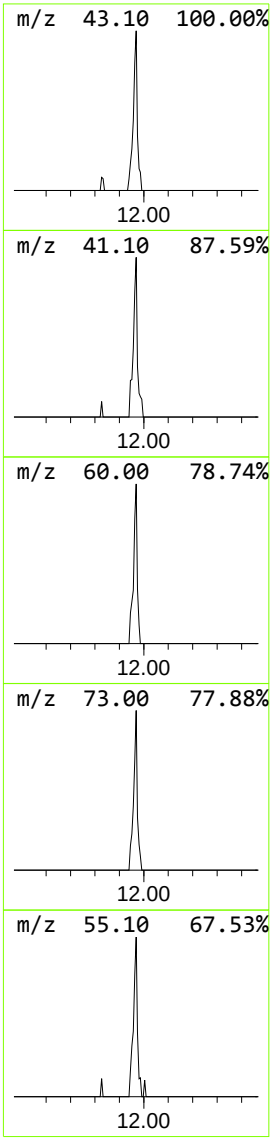
Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	11.51 ng	38130	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





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Sample : M3076-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 20210578-COM-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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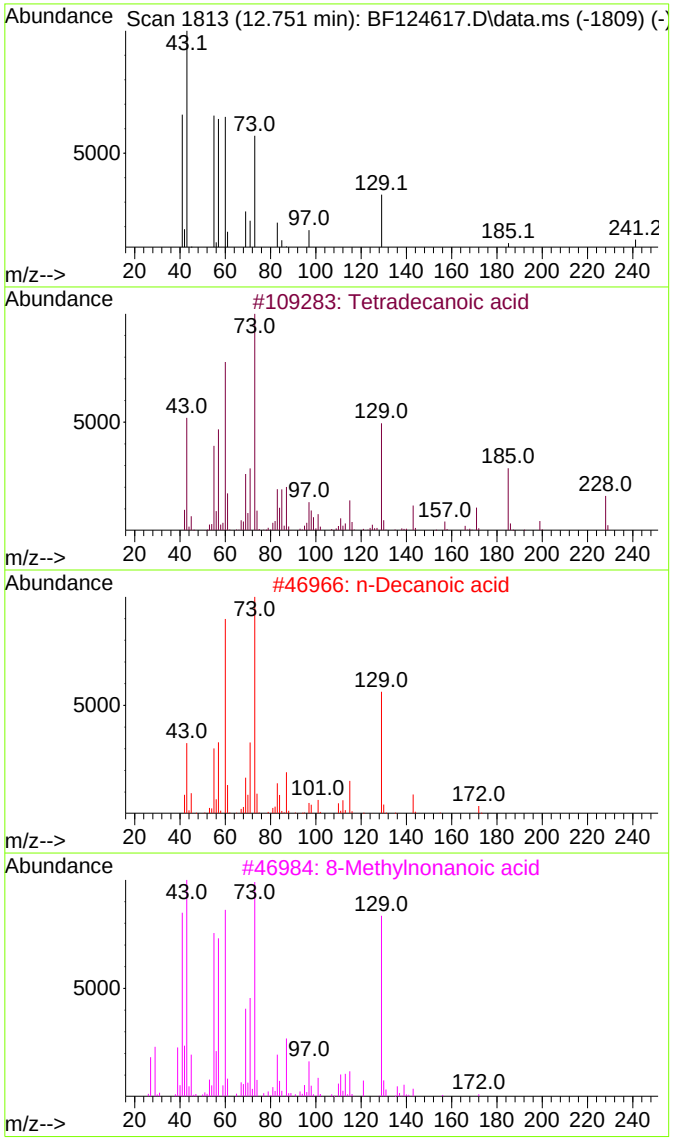
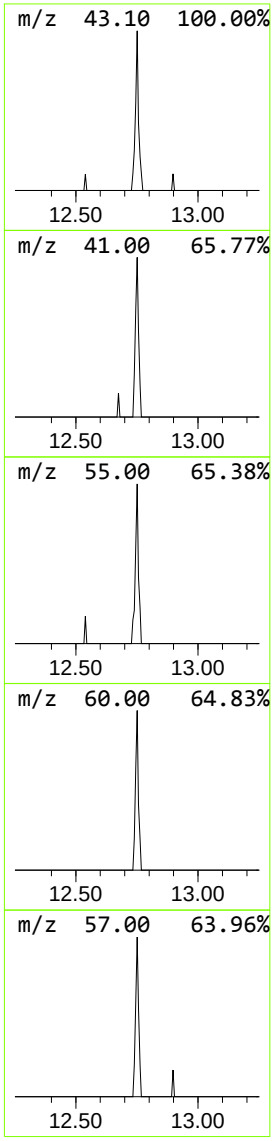
Peak Number 5 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	5.06 ng	16745	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
2	n-Decanoic acid	172	C10H20O2	000334-48-5	50
3	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	43
4	Butyl octacosyl ether	467	C32H66O	1000406-41-1	27
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	27





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Misc :
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Instrument : BNA_F
ClientSampleId : 20210578-COM-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070721.M
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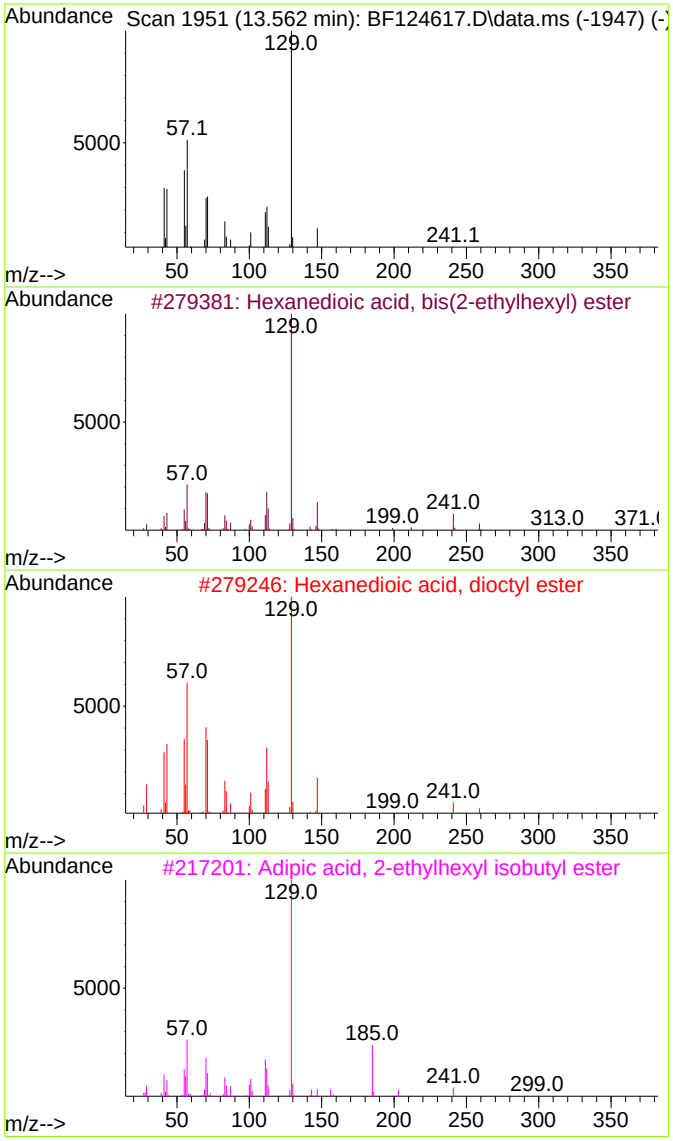
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

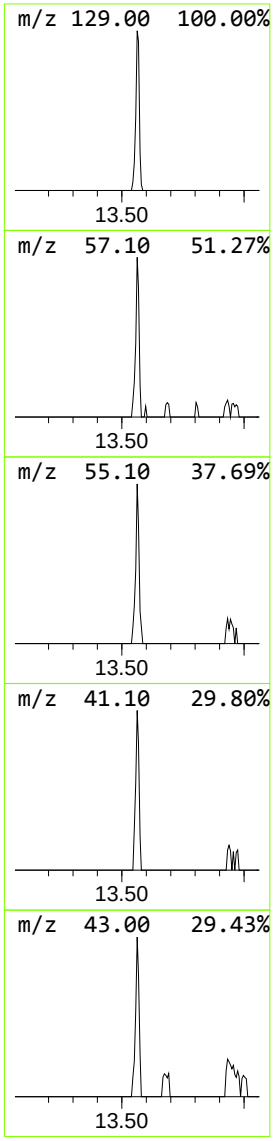
****

Peak Number 6 Hexanedioic acid, bis(2-eth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.563	19.69 ng	39809	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	83
2	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	68
3	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	59
4	Adipic acid, di(oct-4-yl ester)	370	C22H42O4	1000160-80-1	53
5	Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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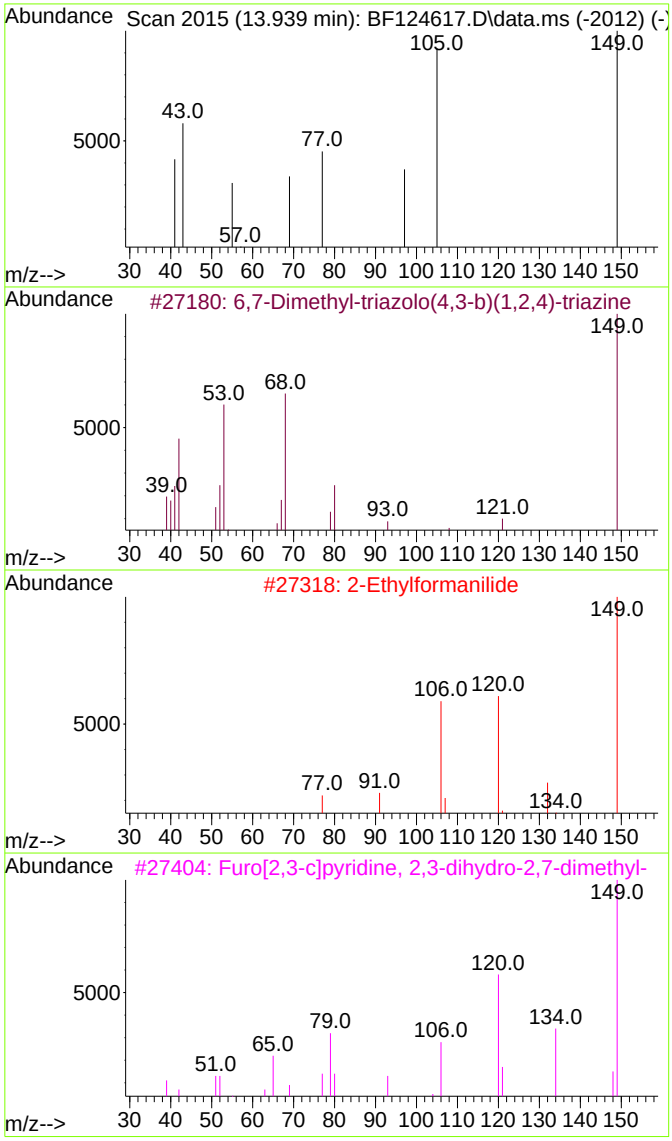
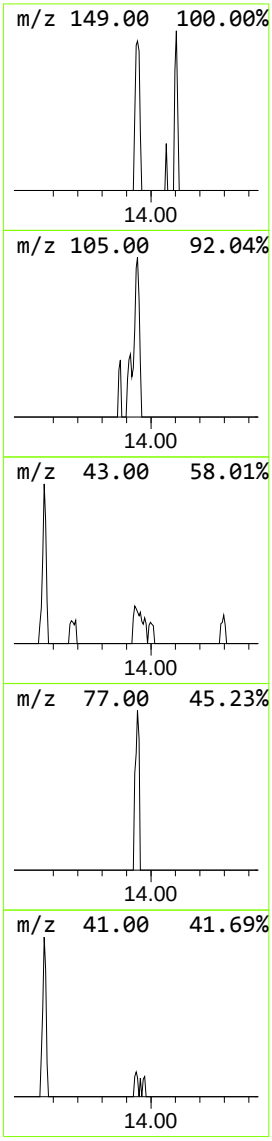
Peak Number 7 unknown13.939 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	3.36 ng	6785	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,7-Dimethyl-triazolo(4,3-b)(1,2...	149	C6H7N5	061139-73-9	2
2	2-Ethylformanilide	149	C9H11NO	002860-30-2	2
3	Furo[2,3-c]pyridine, 2,3-dihydro...	149	C9H11NO	069022-82-8	2
4	Mercaptamine	77	C2H7NS	000060-23-1	2
5	1-Phenylpent-4-en-1-one	160	C11H12O	003240-29-7	2





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.246	9.1	ng	16523	1	6.916	36500	20.0
Ethanol, 2-(2-b...	8.092	10.7	ng	27704	2	8.198	51826	20.0
Phenyl salicylate	11.186	2.5	ng	8136	4	11.445	66230	20.0
n-Hexadecanoic ...	11.969	11.5	ng	38130	4	11.445	66230	20.0
Tetradecanoic acid	12.751	5.1	ng	16745	4	11.445	66230	20.0
Hexanedioic aci...	13.563	19.7	ng	39809	5	14.080	40440	20.0
unknown13.939	13.939	3.4	ng	6785	5	14.080	40440	20.0