

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121022\
 Data File : BP013061.D
 Acq On : 11 Dec 2022 03:49
 Operator : CG/JU
 Sample : N5927-22
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 EXZA8

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % 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_P\Methods\SFAM-EPA-BP120722.M
 Title : SVOA CALIBRATION

Signal : TIC: BP013061.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.352	24	28	40	rVB	157344	234429	0.90%	0.090%
2	3.646	75	78	84	rVB	32434	47637	0.18%	0.018%
3	3.781	98	101	116	rBV	669668	1122425	4.29%	0.430%
4	4.017	136	141	147	rVB	78626	126541	0.48%	0.048%
5	4.111	153	157	163	rVB2	52092	69727	0.27%	0.027%
6	4.652	245	249	258	rVB7	22402	38313	0.15%	0.015%
7	6.199	506	512	519	rVB	25472	44525	0.17%	0.017%
8	6.993	642	647	655	rBV	33084	58558	0.22%	0.022%
9	7.122	663	669	684	rVB	702462	1142013	4.36%	0.437%
10	7.293	691	698	705	rBV	3376204	5269822	20.14%	2.018%
11	7.346	705	707	717	rVB3	72572	124462	0.48%	0.048%
12	7.499	722	733	744	rBV	2952237	4750844	18.16%	1.820%
13	7.969	805	813	819	rBV	2714624	4250923	16.25%	1.628%
14	8.028	819	823	835	rVB	153746	252243	0.96%	0.097%
15	8.675	925	933	945	rBV	2290617	3589072	13.72%	1.375%
16	8.987	980	986	995	rBV2	70282	138992	0.53%	0.053%
17	9.075	997	1001	1004	rVV3	22800	38272	0.15%	0.015%
18	9.140	1004	1012	1018	rVV	3929032	6593555	25.20%	2.525%
19	9.187	1018	1020	1026	rVV3	128606	193005	0.74%	0.074%
20	9.234	1026	1028	1035	rVV5	25281	52429	0.20%	0.020%
21	9.540	1073	1080	1083	rBV2	28278	50920	0.19%	0.020%
22	9.675	1097	1103	1106	rBV	80417	123516	0.47%	0.047%
23	9.710	1106	1109	1119	rVB2	50724	92267	0.35%	0.035%
24	9.863	1127	1135	1147	rBV	3254499	5411943	20.68%	2.073%
25	10.005	1154	1159	1166	rBV5	19655	42080	0.16%	0.016%
26	10.234	1193	1198	1203	rBV3	32404	52957	0.20%	0.020%
27	10.399	1218	1226	1234	rBV	4724369	7848278	29.99%	3.006%
28	10.558	1247	1253	1260	rBV	64154	119791	0.46%	0.046%
29	10.787	1283	1292	1306	rBV	3887350	7095832	27.12%	2.718%
30	10.922	1307	1315	1334	rVB	3664845	6536630	24.98%	2.504%
31	11.563	1420	1424	1429	rBV5	24234	41178	0.16%	0.016%
32	11.728	1444	1452	1458	rBV8	36994	76184	0.29%	0.029%
33	12.040	1495	1505	1514	rVV4	59289	134331	0.51%	0.051%
34	12.252	1535	1541	1548	rBV	272328	454843	1.74%	0.174%
35	12.363	1555	1560	1566	rVB2	98541	154113	0.59%	0.059%
36	12.493	1577	1582	1590	rBV8	36266	69409	0.27%	0.027%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
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37	12.575	1591	1596	1607	rVB8	25654	66011	0.25%	0.025%
38	12.934	1653	1657	1660	rBV3	27125	40171	0.15%	0.015%
39	12.987	1660	1666	1678	rBV2	538793	1235326	4.72%	0.473%
40	13.128	1686	1690	1696	rVB5	43965	61395	0.23%	0.024%
41	13.234	1697	1708	1712	rBV	459785	819981	3.13%	0.314%
42	13.281	1712	1716	1719	rVV	228542	326822	1.25%	0.125%
43	13.363	1722	1730	1739	rVV2	465043	1188003	4.54%	0.455%
44	13.440	1739	1743	1748	rVB3	168473	253753	0.97%	0.097%
45	13.540	1748	1760	1768	rBV	1078931	2028250	7.75%	0.777%
46	13.693	1781	1786	1790	rBV	134094	188277	0.72%	0.072%
47	13.734	1790	1793	1808	rVB9	73447	192144	0.73%	0.074%
48	13.851	1808	1813	1819	rBV6	54674	116231	0.44%	0.045%
49	14.016	1834	1841	1851	rBV	9758040	13604166	51.99%	5.211%
50	14.134	1856	1861	1867	rVB9	40024	83141	0.32%	0.032%
51	14.257	1877	1882	1884	rBV2	115772	187602	0.72%	0.072%
52	14.304	1884	1890	1897	rVB2	11043420	16546989	63.24%	6.338%
53	14.610	1935	1942	1951	rVB	6452934	9451529	36.12%	3.620%
54	14.693	1953	1956	1962	rVB6	27350	47017	0.18%	0.018%
55	14.798	1965	1974	1985	rBV	637836	1061488	4.06%	0.407%
56	14.922	1991	1995	1999	rBV6	28502	45200	0.17%	0.017%
57	15.010	2006	2010	2018	rVB5	62699	107619	0.41%	0.041%
58	15.169	2032	2037	2043	rBV2	76468	142807	0.55%	0.055%
59	15.240	2046	2049	2059	rVB3	62223	119787	0.46%	0.046%
60	15.351	2063	2068	2072	rBV	299097	406218	1.55%	0.156%
61	15.398	2072	2076	2082	rVV2	72485	131432	0.50%	0.050%
62	15.445	2082	2084	2091	rVB2	39698	48621	0.19%	0.019%
63	15.604	2103	2111	2122	rBV	13859833	20723791	79.20%	7.938%
64	15.716	2124	2130	2144	rVV	4918776	6911704	26.41%	2.647%
65	15.840	2147	2151	2157	rVB3	72785	118071	0.45%	0.045%
66	15.963	2168	2172	2176	rBV3	31460	41336	0.16%	0.016%
67	16.004	2176	2179	2183	rVB3	30001	37985	0.15%	0.015%
68	16.240	2215	2219	2221	rBV3	27184	36914	0.14%	0.014%
69	16.281	2222	2226	2229	rVV2	56061	85079	0.33%	0.033%
70	16.310	2229	2231	2238	rVV6	49688	101711	0.39%	0.039%
71	16.387	2240	2244	2249	rVB6	37345	55700	0.21%	0.021%
72	16.492	2258	2262	2268	rBV3	42503	76007	0.29%	0.029%
73	16.745	2302	2305	2308	rVB4	31610	36702	0.14%	0.014%
74	16.828	2316	2319	2326	rVB9	39504	66413	0.25%	0.025%
75	17.110	2363	2367	2370	rVV3	51470	63028	0.24%	0.024%
76	17.163	2371	2376	2383	rVB5	64349	110911	0.42%	0.042%

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77	17.269	2390	2394	2399	rVB2	93716	120410	0.46%	0.046%
78	17.363	2404	2410	2417	rBV	8290652	11695759	44.70%	4.480%
79	17.463	2421	2427	2440	rVB2	14900332	22441448	85.76%	8.596%
80	17.645	2454	2458	2468	rBV	98973	179974	0.69%	0.069%
81	17.739	2472	2474	2478	rVB4	30303	34915	0.13%	0.013%
82	18.022	2518	2522	2526	rVB	112710	147630	0.56%	0.057%
83	18.234	2553	2558	2567	rBV	1144612	1505851	5.75%	0.577%
84	18.310	2567	2571	2575	rVB	164144	215210	0.82%	0.082%
85	18.645	2625	2628	2633	rVB4	50714	56310	0.22%	0.022%
86	18.969	2681	2683	2688	rVB	74772	82829	0.32%	0.032%
87	19.057	2695	2698	2702	rBV2	87318	110734	0.42%	0.042%
88	19.269	2730	2734	2738	rBV	250698	326041	1.25%	0.125%
89	19.339	2742	2746	2749	rBV	227642	294999	1.13%	0.113%
90	19.463	2763	2767	2773	rBV	486227	662641	2.53%	0.254%
91	19.692	2800	2806	2814	rBV	18708652	26166476	100.00%	10.022%
92	21.139	3048	3052	3064	rBV	1036821	1607752	6.14%	0.616%
93	21.339	3083	3086	3092	rVB	363286	394695	1.51%	0.151%
94	21.451	3099	3105	3115	rBV	8827107	12158576	46.47%	4.657%
95	22.575	3293	3296	3303	rVB	285863	413267	1.58%	0.158%
96	23.145	3390	3393	3400	rVB	391449	600998	2.30%	0.230%
97	23.780	3492	3501	3518	rVV2	11078457	24071398	91.99%	9.220%
98	23.939	3520	3528	3540	rVB2	5380324	11090675	42.39%	4.248%
99	24.563	3629	3634	3642	rVB	484366	977900	3.74%	0.375%
100	28.092	4224	4234	4252	rVB	3571103	12315951	47.07%	4.717%

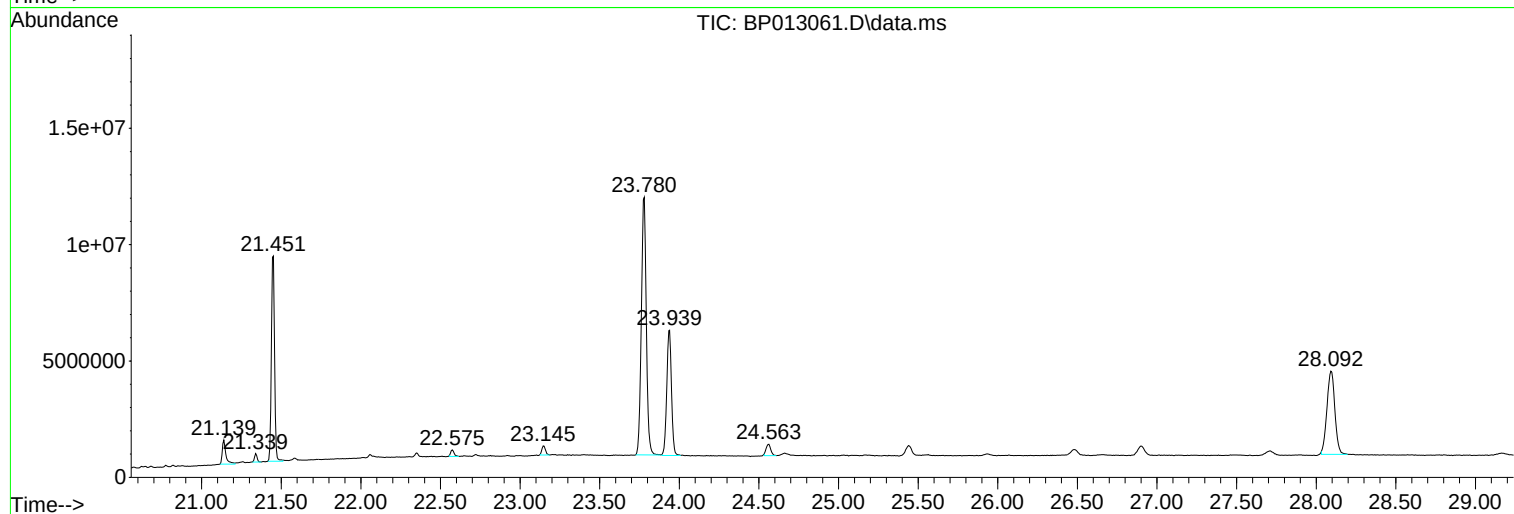
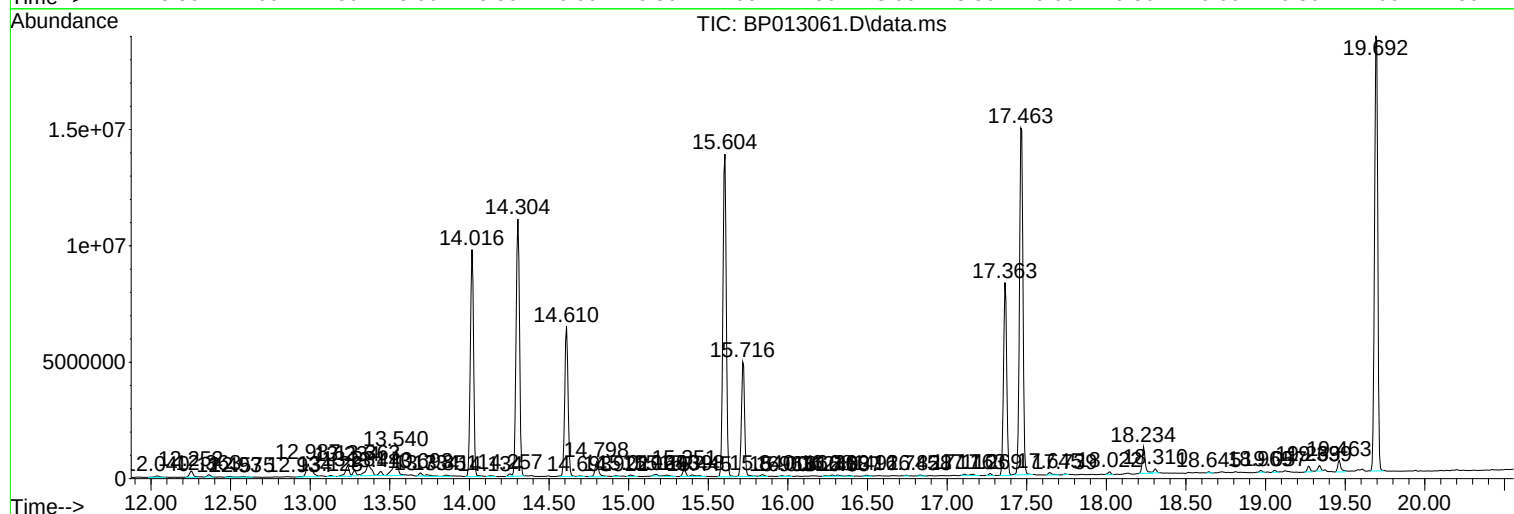
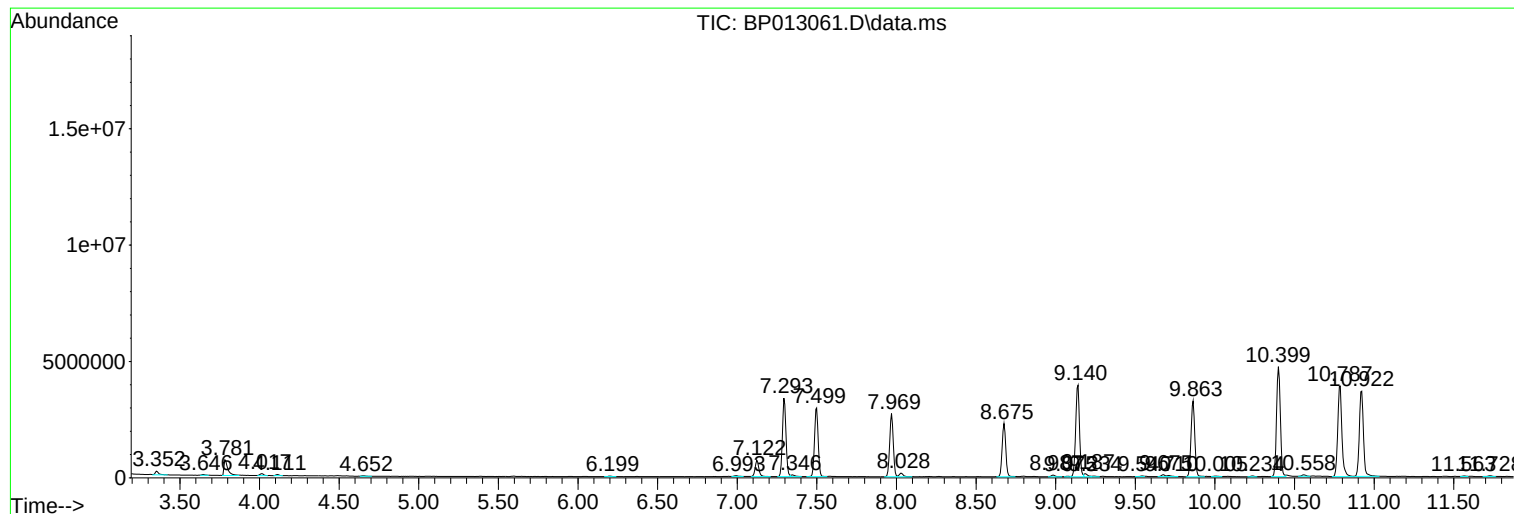
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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



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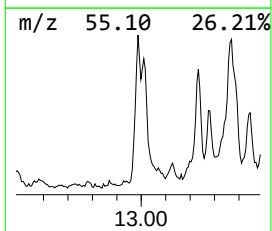
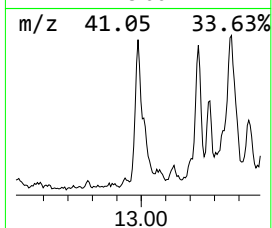
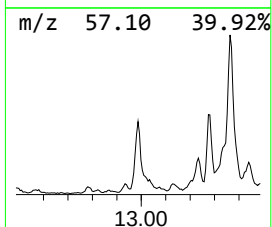
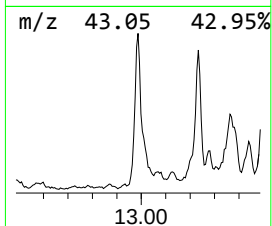
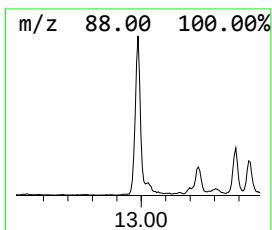
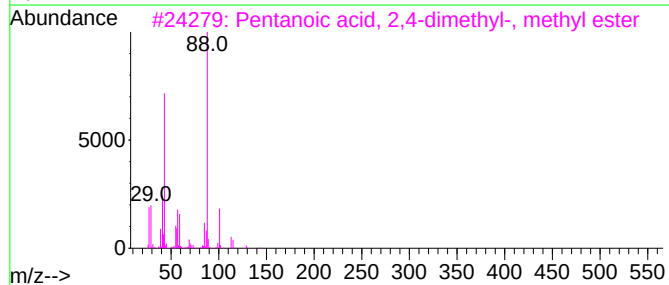
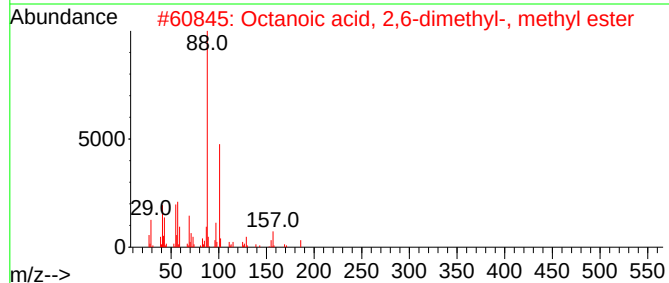
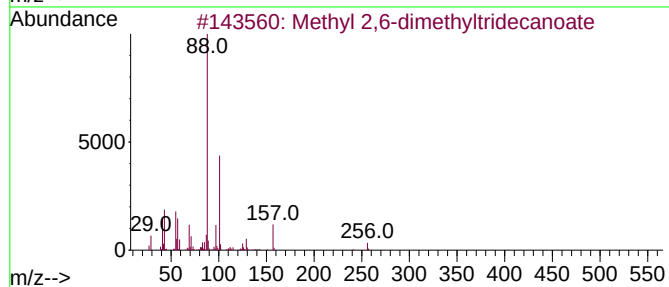
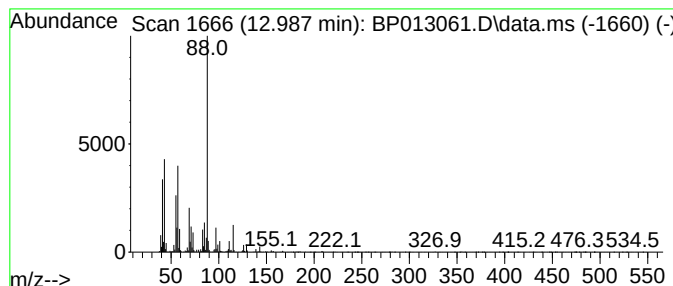
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Methyl 2,6-dimethyltridecan... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.987	2.61 ng/ul	1235330	Acenaphthene-d10	14.610	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 2,6-dimethyltridecanoate	256	C16H32O2	073105-76-7	53
2	Octanoic acid, 2,6-dimethyl-, me...	186	C11H22O2	054798-85-5	53
3	Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	52
4	9-Decenoic acid, 2,4-dimethyl-, ...	212	C13H24O2	031183-23-0	50
5	Octanoic acid, 2-methyl-, methyl...	172	C10H20O2	002177-86-8	47



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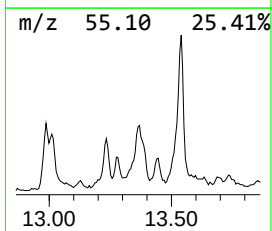
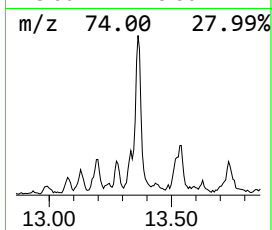
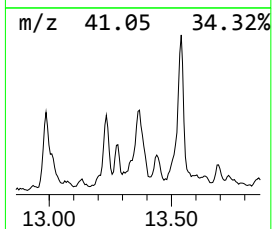
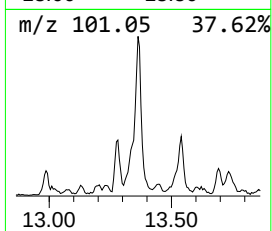
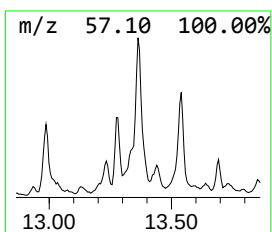
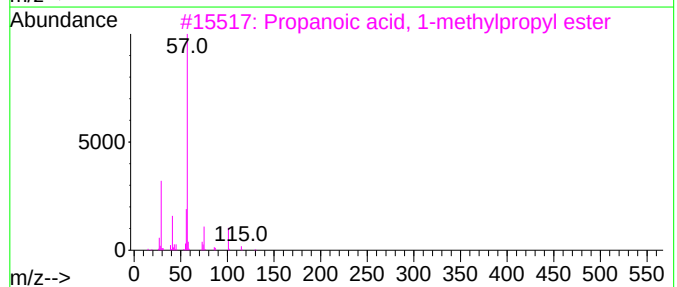
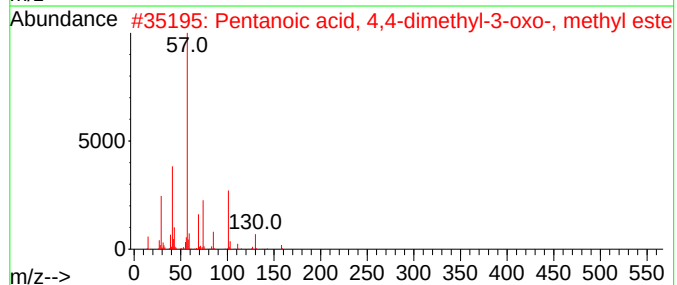
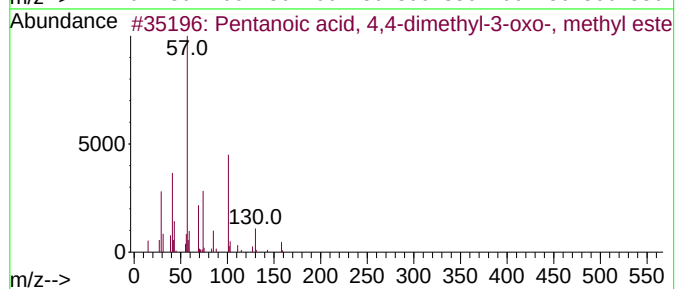
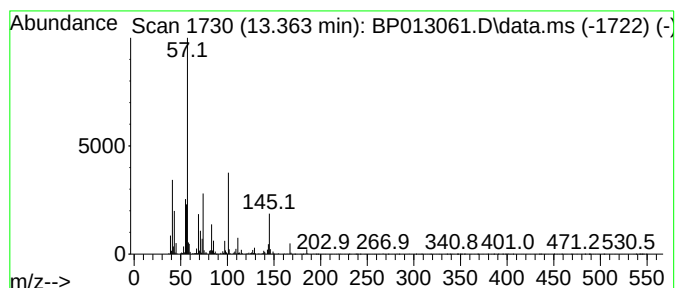
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.363	2.51 ng/ul	1188000	Acenaphthene-d10	14.610	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 4,4-dimethyl-3-o...	158	C8H14O3	055107-14-7	37
2	Pentanoic acid, 4,4-dimethyl-3-o...	158	C8H14O3	055107-14-7	37
3	Propanoic acid, 1-methylpropyl e...	130	C7H14O2	000591-34-4	35
4	1-Methyl-3-pyrrolidinol	101	C5H11NO	013220-33-2	22
5	1-Methyl-3-pyrrolidinol	101	C5H11NO	013220-33-2	22



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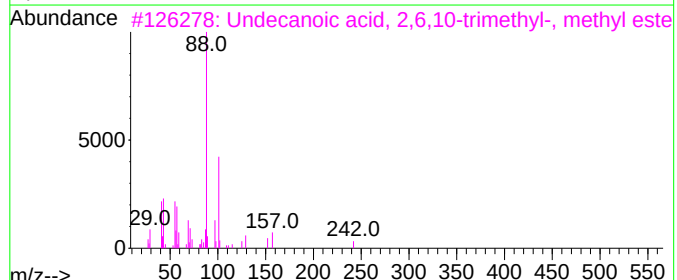
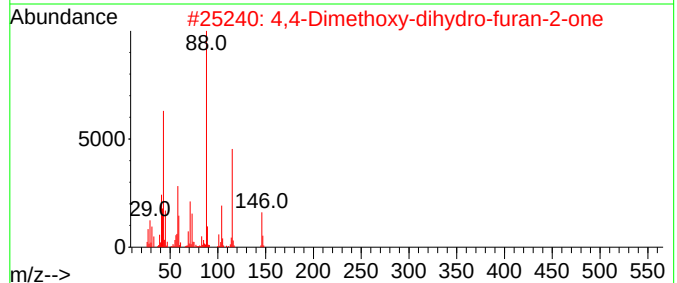
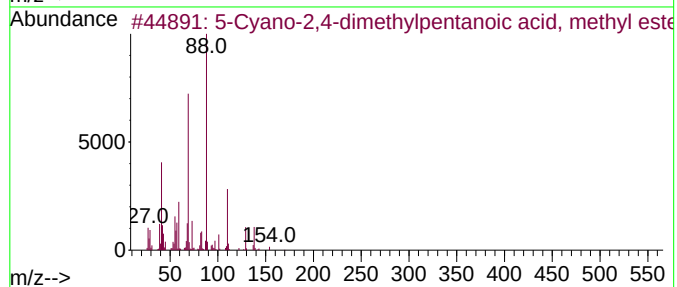
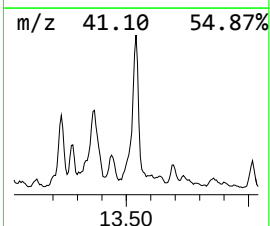
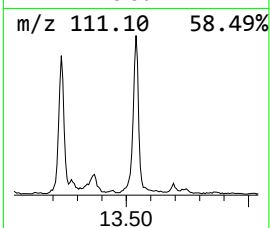
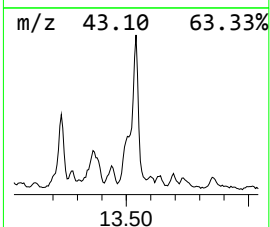
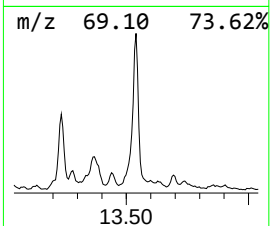
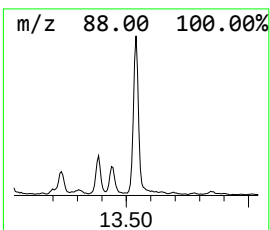
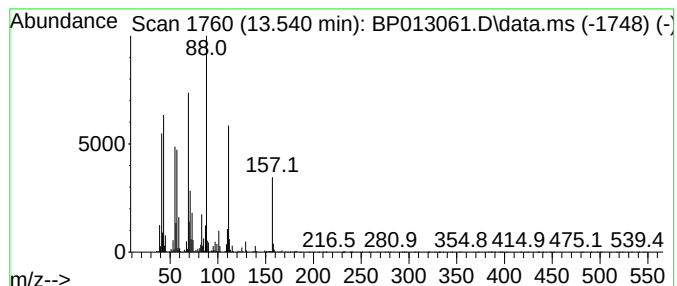
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.540	4.29 ng/ul	2028250	Acenaphthene-d10	14.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Cyano-2,4-dimethylpentanoic ac...	169	C9H15NO2	1000187-83-9	38
2			4,4-Dimethoxy-dihydro-furan-2-one	146	C6H10O4	1000187-47-7	35
3			Undecanoic acid, 2,6,10-trimethy...	242	C15H30O2	001001-79-2	35
4			Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	27
5			Heptanoic acid, 2-methyl-, methy...	158	C9H18O2	051209-78-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121022\
Data File : BP013061.D
Acq On : 11 Dec 2022 03:49
Operator : CG/JU
Sample : N5927-22
Misc :
ALS Vial : 32 Sample Multiplier: 1

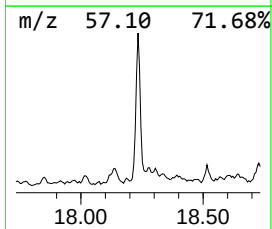
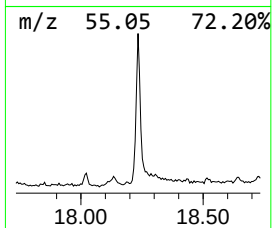
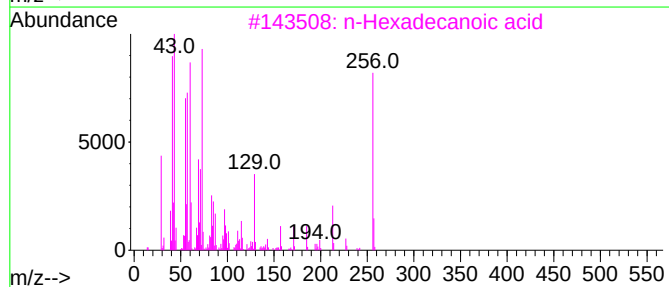
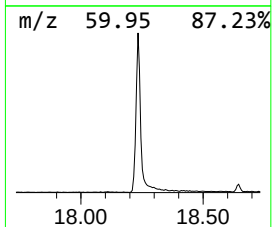
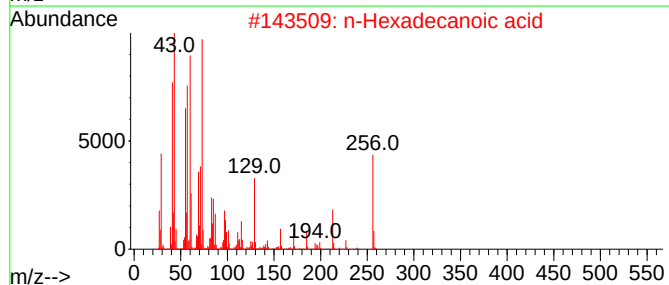
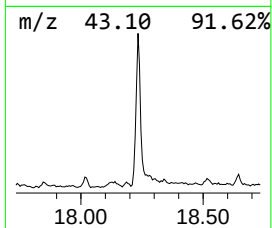
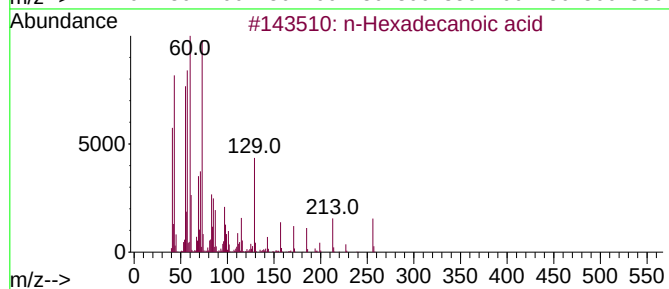
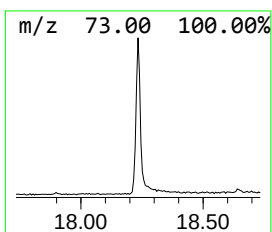
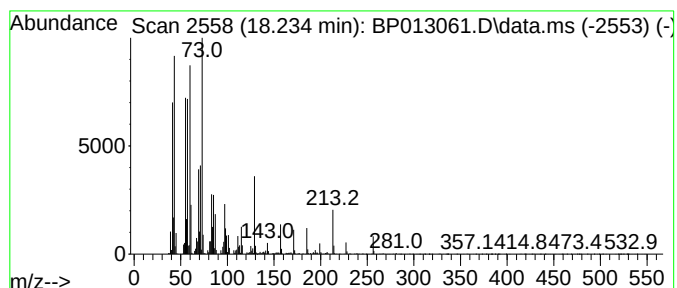
Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.234	2.58 ng/ul	1505850	Phenanthrene-d10	17.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121022\
Data File : BP013061.D
Acq On : 11 Dec 2022 03:49
Operator : CG/JU
Sample : N5927-22
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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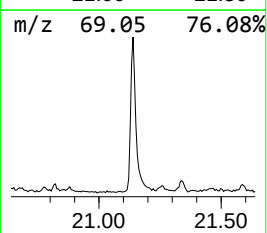
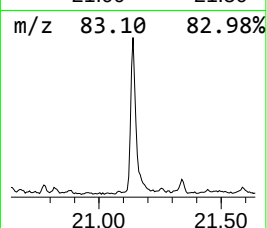
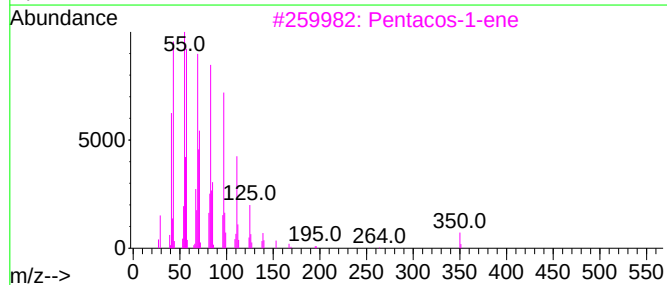
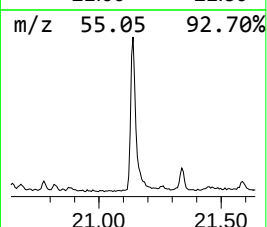
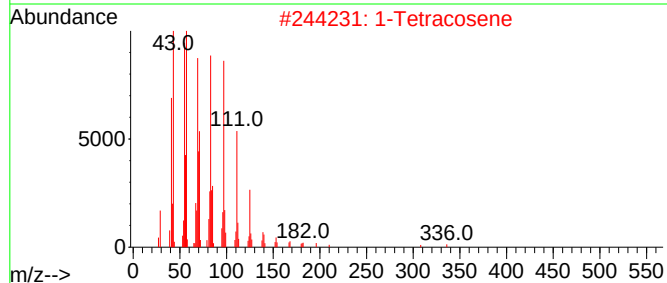
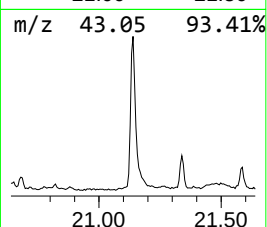
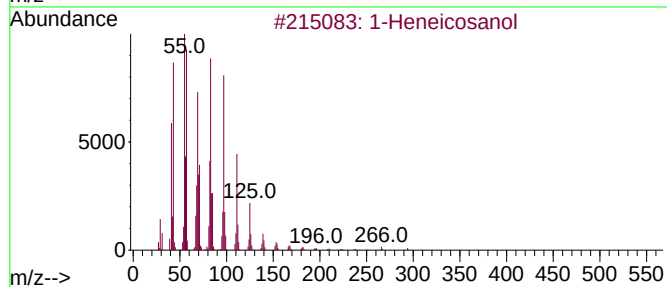
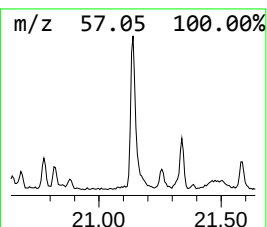
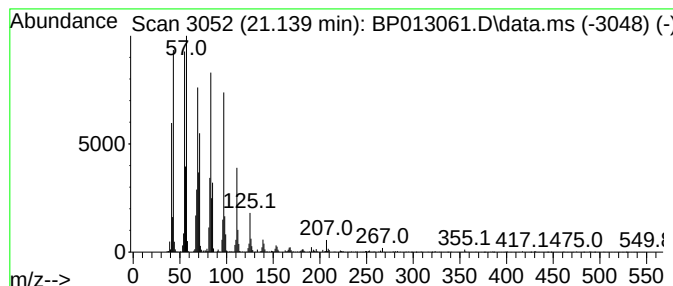
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.139	2.64 ng/ul	1607750	Chrysene-d12	21.451

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		1-Tetracosene	336	C24H48	010192-32-2	94
3		Pentacos-1-ene	350	C25H50	016980-85-1	94
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5		1-Hexacosene	364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121022\
Data File : BP013061.D
Acq On : 11 Dec 2022 03:49
Operator : CG/JU
Sample : N5927-22
Misc :
ALS Vial : 32 Sample Multiplier: 1

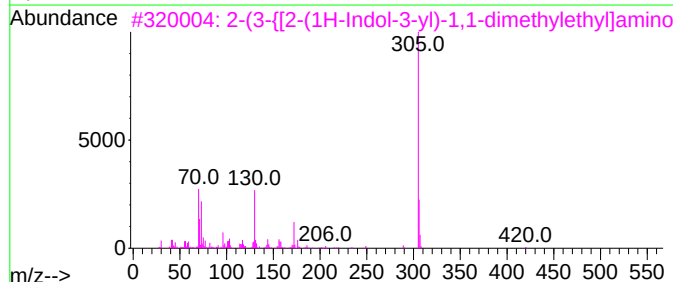
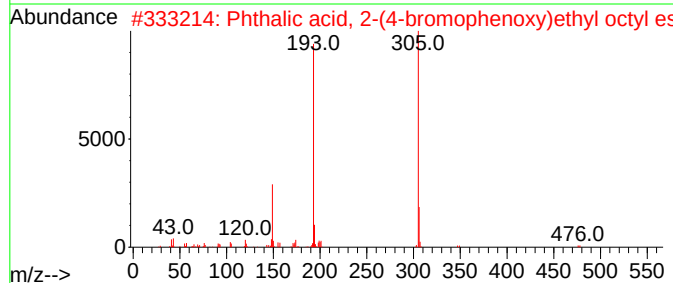
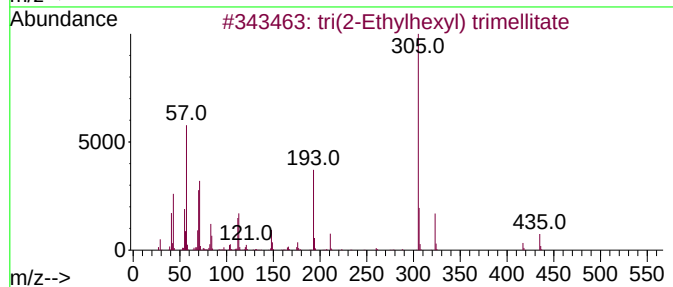
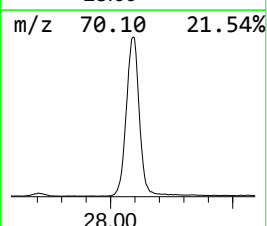
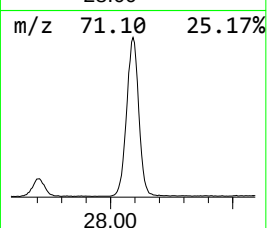
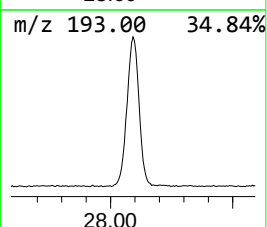
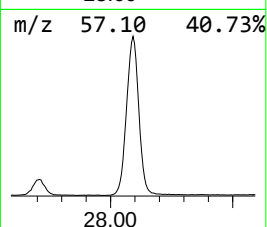
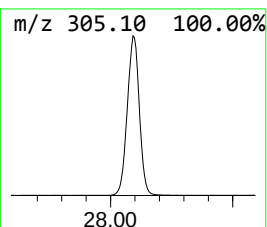
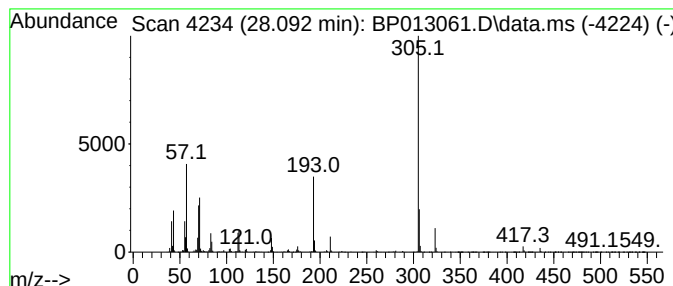
Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 tri(2-Ethylhexyl) trimellitate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.092	22.21 ng/ul	12316000	Perylene-d12	23.939	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	tri(2-Ethylhexyl) trimellitate	546	C33H54O6	003319-31-1	70
2	Phthalic acid, 2-(4-bromophenoxy)ethyl octyl ester	476	C24H29BrO5	1010382-89-7	50
3	2-(3-{[2-(1H-Indol-3-yl)-1,1-dimethylethyl]amino}propyl)-1H-imidazole-4-carboxylic acid	435	C25H33N3O2Si	1000408-41-9	33
4	4-(3-Amino-1-benzofuran-2-yl)-6-methyl-1H-imidazole	305	C19H15NO3	1000410-24-2	32
5	Furo[2,3-H]coumarine, 6-methyl-1H-imidazole	305	C19H15NO3	1000270-15-3	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121022\
Data File : BP013061.D
Acq On : 11 Dec 2022 03:49
Operator : CG/JU
Sample : N5927-22
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EXZA8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA 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
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unknown-01	13.363	2.5	ng/ul	1188000	3	14.610	9451530	20.0
unknown-02	13.540	4.3	ng/ul	2028250	3	14.610	9451530	20.0
n-Hexadecanoic ...	18.234	2.6	ng/ul	1505850	4	17.363	11695800	20.0
1-Heneicosanol	21.139	2.6	ng/ul	1607750	5	21.451	12158600	20.0
tri(2-Ethylhexy...	28.092	22.2	ng/ul	12316000	6	23.939	11090700	20.0